# Full wwPDB EM Validation Report ⓘ

Jan 7, 2023 – 10:39 am GMT

| | | |
|---|---|---|
| PDB ID | : | 7NWH |
| EMDB ID | : | EMD-12632 |
| Title | : | Mammalian pre-termination 80S ribosome with eRF1 and eRF3 bound by Blasticidin S. |
| Authors | : | Powers, K.T.; Yadav, S.K.N.; Bufton, J.C.; Schaffitzel, C. |
| Deposited on | : | 2021-03-16 |
| Resolution | : | 4.10 Å(reported) |
| Based on initial model | : | 5LZT |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references ⓘ) were used in the production of this report:

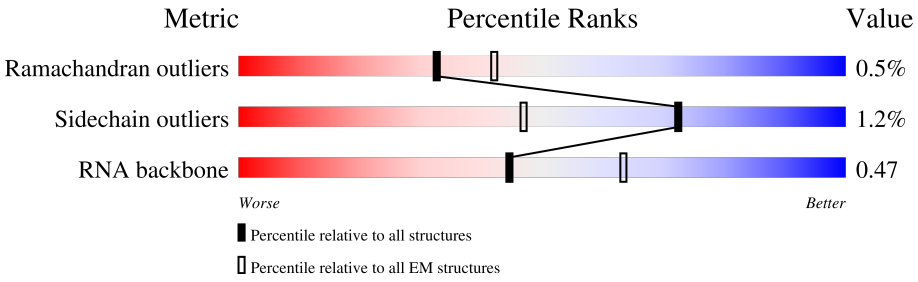
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 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 4.10 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 249 | 95% |
| 2 | C | 378 | 92% |
| 3 | d | 108 | 93% 6% |
| 4 | DD | 281 | 47% 78% 19% |
| 5 | dd | 56 | 46% 98% |
| 6 | D | 296 | 98% |
| 7 | e | 129 | 96% |
| 8 | EE | 263 | 20% 98% |

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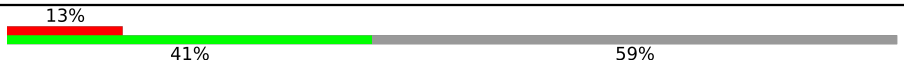
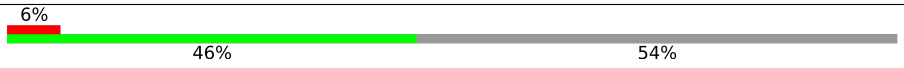
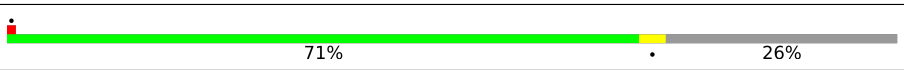
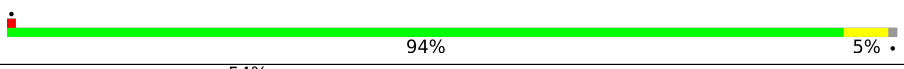
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | ee | 133 |   |
| 10 | b | 226 |   |
| 11 | E | 291 |   |
| 12 | f | 110 |   |
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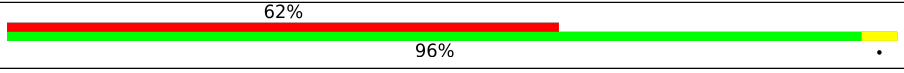
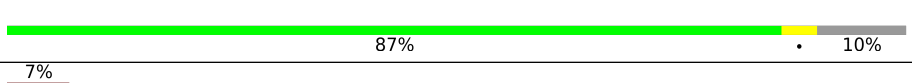
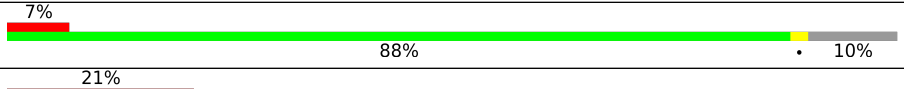
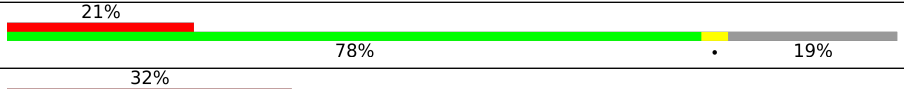
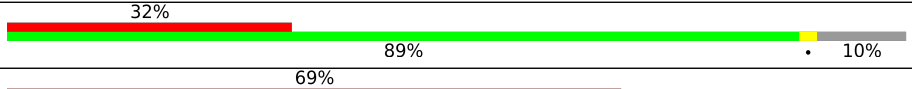
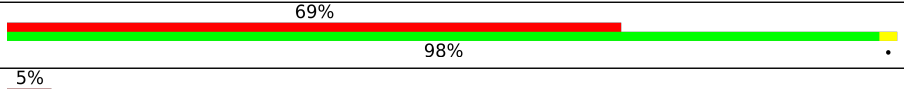
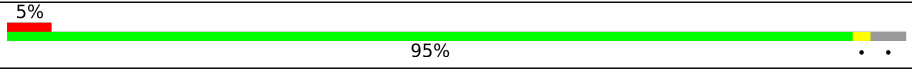
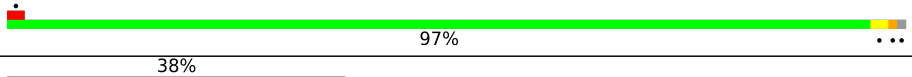
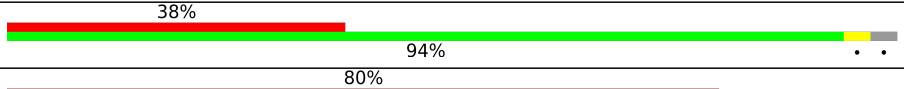
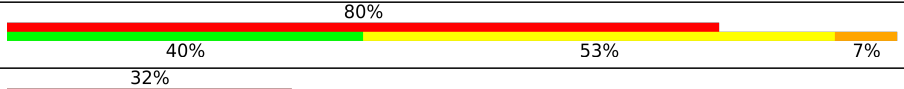
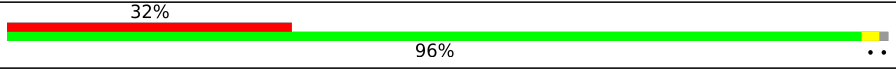
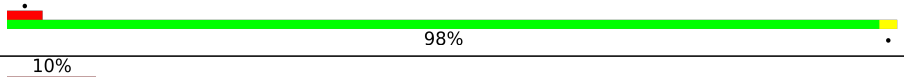
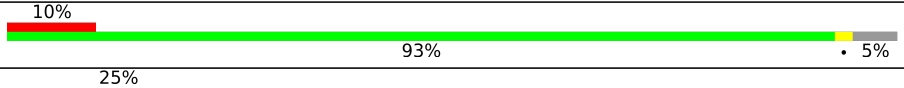
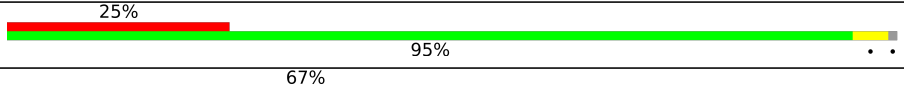
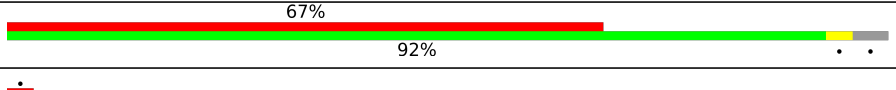
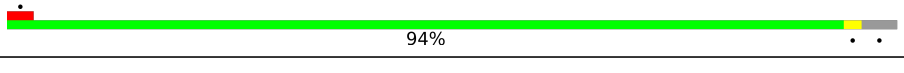
| 14 | ff | 68 |   |
| 15 | F | 249 |   |
| 16 | g | 126 |   |
| 17 | BB | 264 |   |
| 18 | GG | 263 |   |
| 19 | gg | 314 |   |
| 20 | G | 242 |   |
| 21 | h | 123 |   |
| 22 | HH | 191 |   |
| 23 | hh | 15 |   |
| 24 | bb | 84 |   |
| 25 | H | 190 |   |
| 26 | i | 107 |   |
| 27 | II | 208 |   |
| 28 | ii | 437 |   |
| 29 | I | 214 |   |
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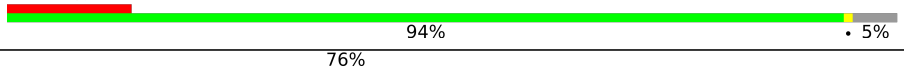
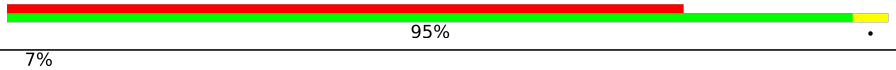
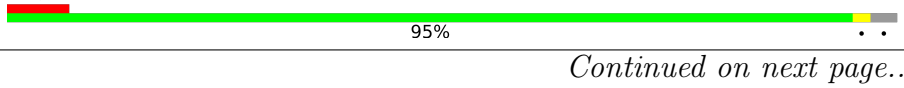
| 31 | JJ | 194 |   |
| 32 | jj | 428 |   |
| 33 | J | 176 |   |

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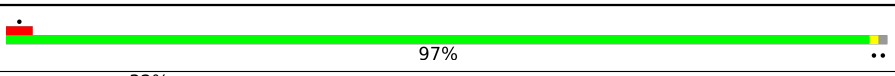
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | k | 70 |   |
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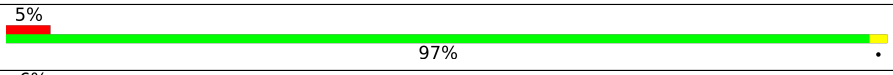
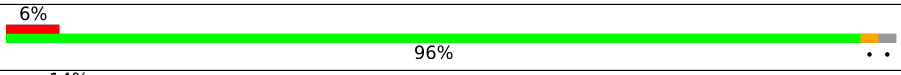
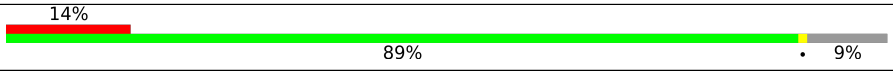
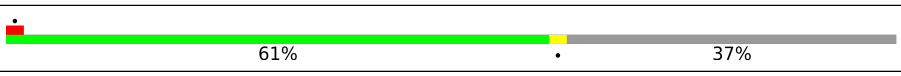
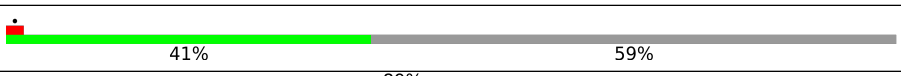
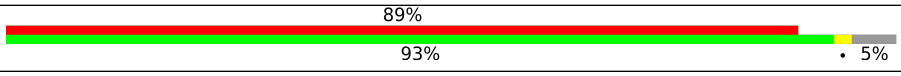
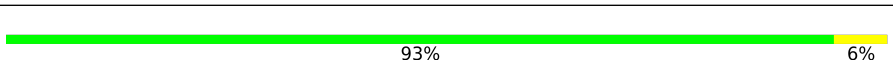
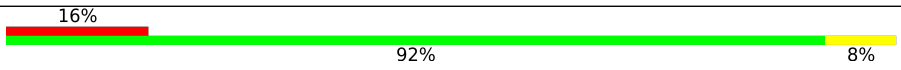
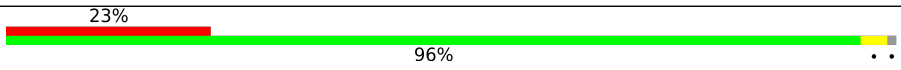
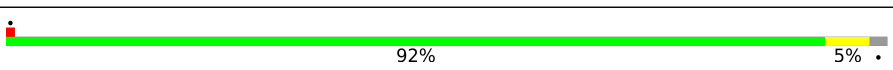
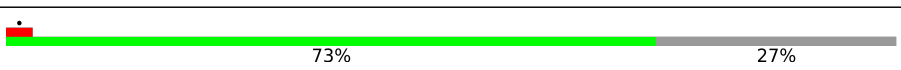
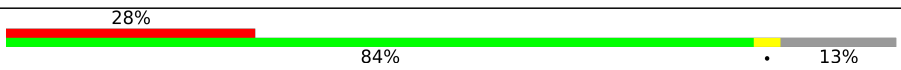
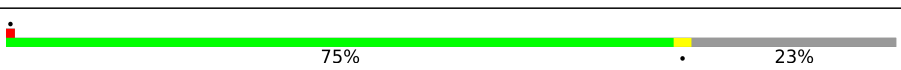
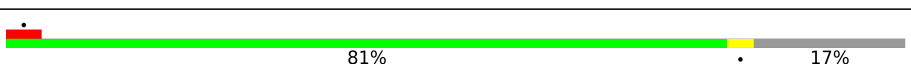
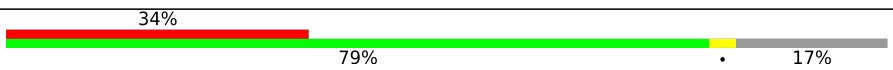
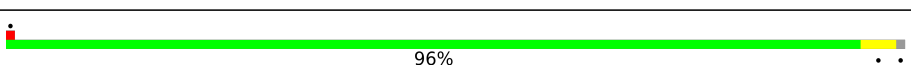
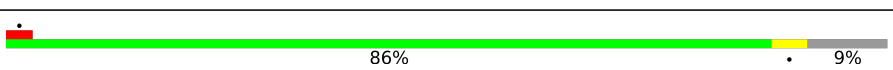
| 36 | L | 211 |   |
| 37 | l | 51 |   |
| 38 | LL | 158 |   |
| 39 | M | 218 |   |
| 40 | m | 128 |   |
| 41 | MM | 123 |   |
| 42 | N | 204 |   |
| 43 | n | 25 |   |
| 44 | NN | 150 |   |
| 45 | O | 203 |   |
| 46 | o | 142 |   |
| 47 | OO | 156 |   |
| 48 | P | 199 |   |
| 49 | p | 109 |   |
| 50 | PP | 145 |   |
| 51 | Q | 188 |   |
| 52 | r | 137 |   |
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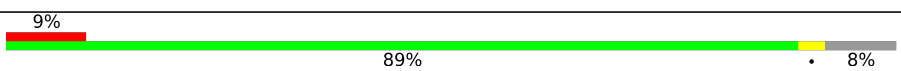
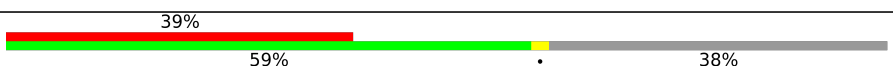
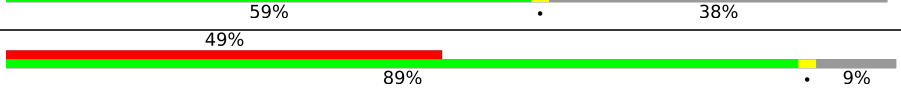
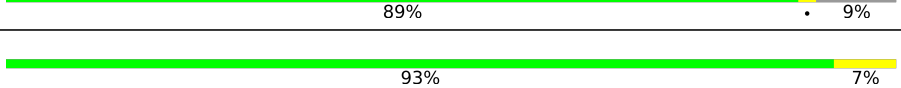
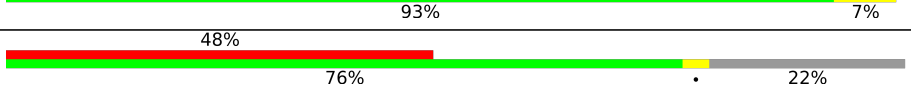
| 54 | R | 196 |   |
| 55 | s | 318 |   |
| 56 | RR | 145 |   |
| 57 | S | 176 |   |
| 58 | t | 196 |   |

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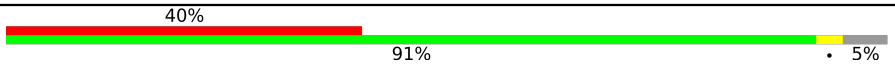
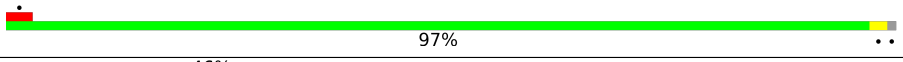
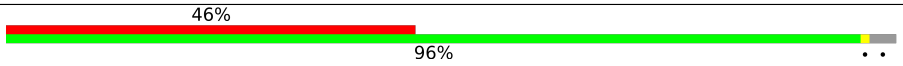
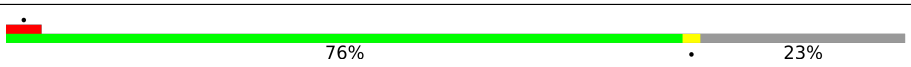
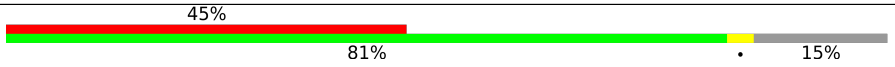
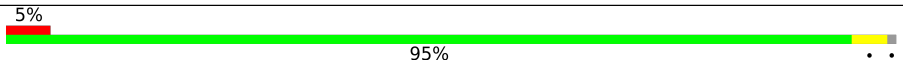
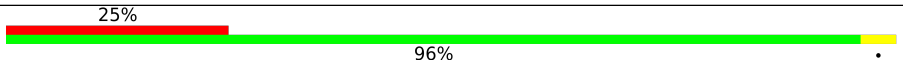
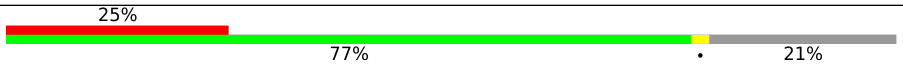
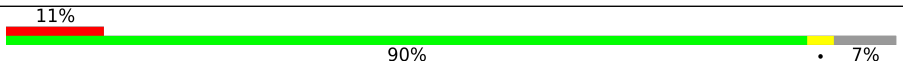
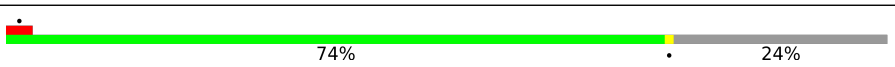
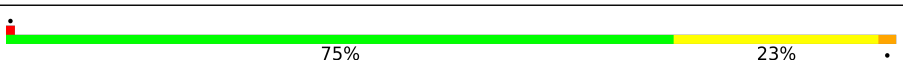
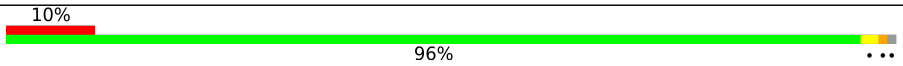
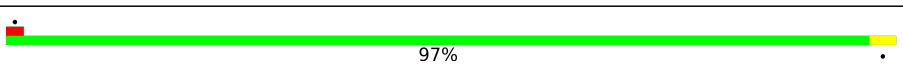
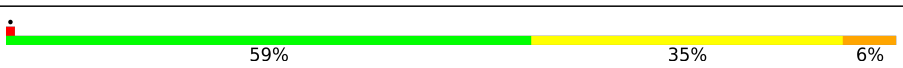
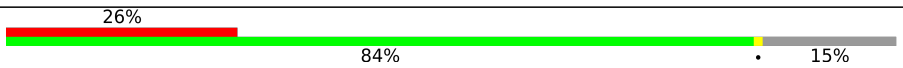
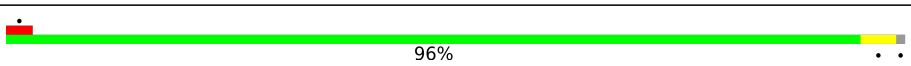
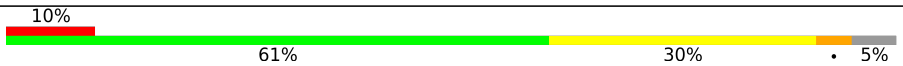
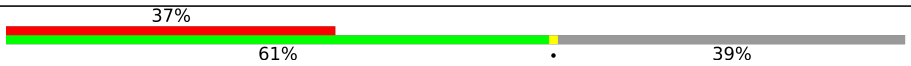
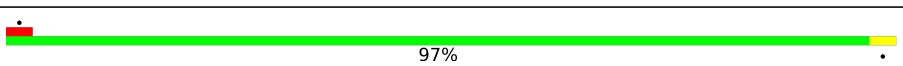
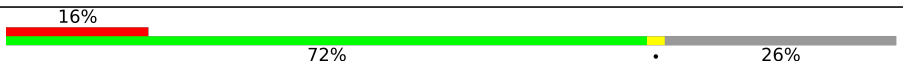
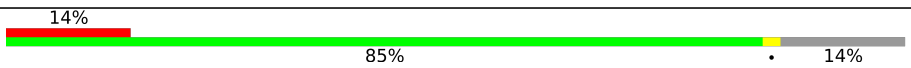
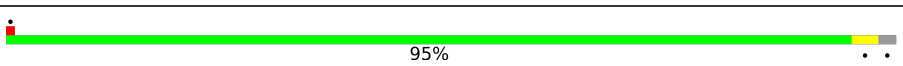
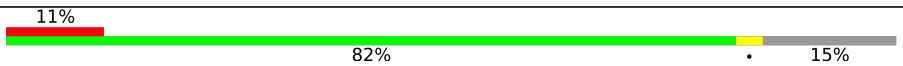
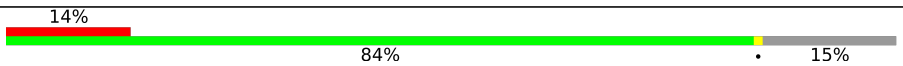
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 59 | SS | 152 |   |
| 60 | T | 160 |   |
| 61 | TT | 145 |   |
| 62 | U | 128 |   |
| 63 | UU | 118 |   |
| 64 | V | 132 |   |
| 65 | VV | 83 |   |
| 66 | W | 134 |   |
| 67 | 5 | 3705 |   |
| 68 | WW | 139 |   |
| 69 | X | 156 |   |
| 70 | 7 | 120 |   |
| 71 | XX | 142 |   |
| 72 | Y | 134 |   |
| 73 | 8 | 151 |   |
| 74 | YY | 146 |   |
| 75 | Z | 136 |   |
| 76 | 9 | 1779 |   |
| 77 | ZZ | 122 |   |
| 78 | a | 147 |   |
| 79 | AA | 295 |   |
| 80 | aa | 117 |   |
| 81 | B | 402 |   |
| 82 | c | 115 |   |
| 83 | CC | 259 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 84 | cc | 69 |   |

# 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 385116 atoms, of which 165738 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 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | A | 248 | 3891 | 1189 | 1993 | 389 | 314 | 6 | 0 | 0 |

- Molecule 2 is a protein called uL4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | C | 362 | 5936 | 1812 | 3053 | 577 | 480 | 14 | 0 | 0 |

- Molecule 3 is a protein called eL31.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 3 | d | 107 | 1818 | 560 | 930 | 171 | 155 | 2 | 0 | 0 |

- Molecule 4 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 4 | DD | 228 | 3632 | 1126 | 1864 | 318 | 316 | 8 | 0 | 0 |

- Molecule 5 is a protein called S29.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 5 | dd | 55 | 908 | 286 | 449 | 94 | 74 | 5 | 0 | 0 |

- Molecule 6 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 6 | D | 293 | 4815 | 1512 | 2424 | 438 | 427 | 14 | 0 | 0 |

- Molecule 7 is a protein called Ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | e | 128 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2200 | 667 | 1147 | 216 | 165 | 5 | | |

- Molecule 8 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | EE | 262 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4253 | 1324 | 2177 | 386 | 358 | 8 | | |

- Molecule 9 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | ee | 55 | Total | C | H | N | O | S | 0 | 0 |
| | | | 935 | 274 | 492 | 97 | 71 | 1 | | |

- Molecule 10 is a protein called eL29.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | b | 104 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1768 | 527 | 920 | 189 | 129 | 3 | | |

- Molecule 11 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | E | 216 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3617 | 1115 | 1888 | 329 | 282 | 3 | | |

- Molecule 12 is a protein called eL33.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | f | 109 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1788 | 555 | 912 | 174 | 143 | 4 | | |

- Molecule 13 is a protein called Ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | FF | 185 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2993 | 921 | 1522 | 277 | 266 | 7 | | |

- Molecule 14 is a protein called 40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | ff | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1120 | 351 | 565 | 103 | 94 | 7 | | |

- Molecule 15 is a protein called uL30.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | F | 225 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3870 | 1205 | 1995 | 358 | 303 | 9 | | |

- Molecule 16 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | g | 114 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1905 | 566 | 999 | 187 | 147 | 6 | | |

- Molecule 17 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | BB | 213 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3532 | 1098 | 1803 | 309 | 308 | 14 | | |

- Molecule 18 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | GG | 237 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4005 | 1200 | 2082 | 387 | 329 | 7 | | |

- Molecule 19 is a protein called Epididymis tissue sperm binding protein Li 3a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | gg | 313 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4830 | 1535 | 2394 | 424 | 465 | 12 | | |

- Molecule 20 is a protein called L7a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | G | 233 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3906 | 1199 | 2027 | 361 | 315 | 4 | | |

- Molecule 21 is a protein called uL29.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | h | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2160 | 640 | 1147 | 204 | 168 | 1 | | |

- Molecule 22 is a protein called S7.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | HH | 185 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3070 | 952 | 1582 | 271 | 264 | 1 | | |

- Molecule 23 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | hh | 15 | Total | C | H | N | O | P | 0 | 0 |
| | | | 478 | 142 | 161 | 54 | 106 | 15 | | |

- Molecule 24 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | bb | 83 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1323 | 408 | 672 | 121 | 115 | 7 | | |

- Molecule 25 is a protein called L9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | H | 190 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3113 | 954 | 1597 | 284 | 272 | 6 | | |

- Molecule 26 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | i | 102 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1746 | 520 | 916 | 176 | 129 | 5 | | |

- Molecule 27 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | II | 206 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3459 | 1058 | 1773 | 332 | 291 | 5 | | |

- Molecule 28 is a protein called Eukaryotic peptide chain release factor subunit 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | ii | 419 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6638 | 2104 | 3331 | 562 | 629 | 12 | | |

- Molecule 29 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | I | 205 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3376 | 1056 | 1712 | 321 | 274 | 13 | | |

- Molecule 30 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | j | 86 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1442 | 434 | 737 | 155 | 111 | 5 | | |

- Molecule 31 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | JJ | 185 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3165 | 969 | 1640 | 306 | 248 | 2 | | |

- Molecule 32 is a protein called eRF3a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | jj | 428 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6787 | 2144 | 3419 | 580 | 623 | 21 | | |

- Molecule 33 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | J | 170 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2761 | 861 | 1399 | 254 | 241 | 6 | | |

- Molecule 34 is a protein called L38.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | k | 69 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1206 | 366 | 637 | 103 | 99 | 1 | | |

- Molecule 35 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | KK | 96 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1646 | 530 | 836 | 143 | 131 | 6 | | |

- Molecule 36 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | L | 210 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3522 | 1065 | 1820 | 354 | 279 | 4 | | |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | l | 50 | Total | C | H | N | O | S | 0 | 0 |
| | | | 927 | 286 | 480 | 96 | 64 | 1 | | |

- Molecule 38 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | LL | 143 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2425 | 749 | 1250 | 222 | 198 | 6 | | |

- Molecule 39 is a protein called Ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | M | 138 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2348 | 727 | 1211 | 221 | 182 | 7 | | |

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN EL40.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | m | 52 | Total | C | H | N | O | S | 0 | 0 |
| | | | 894 | 266 | 465 | 90 | 67 | 6 | | |

- Molecule 41 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | MM | 117 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1847 | 570 | 939 | 161 | 169 | 8 | | |

- Molecule 42 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | N | 203 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3451 | 1072 | 1750 | 359 | 266 | 4 | | |

- Molecule 43 is a protein called 60s ribosomal protein l41.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | n | 25 | Total | C | H | N | O | S | 0 | 0 |
| | | | 525 | 145 | 286 | 64 | 27 | 3 | | |

- Molecule 44 is a protein called ribosomal protein uS15.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | NN | 149 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2491 | 770 | 1289 | 228 | 203 | 1 | | |

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN UL13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | O | 199 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3408 | 1051 | 1778 | 319 | 255 | 5 | | |

- Molecule 46 is a protein called eL42.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 46 | o | 104 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1771 | 533 | 920 | 174 | 138 | 6 | | |

- Molecule 47 is a protein called uS11.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | OO | 136 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2055 | 621 | 1039 | 199 | 190 | 6 | | |

- Molecule 48 is a protein called uL22.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | P | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2516 | 777 | 1274 | 241 | 215 | 9 | | |

- Molecule 49 is a protein called ribosomal protein eL43.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 49 | p | 91 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1466 | 445 | 758 | 136 | 120 | 7 | | |

- Molecule 50 is a protein called 40S ribosomal protein uS19.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | PP | 120 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2042 | 635 | 1045 | 187 | 168 | 7 | | |

- Molecule 51 is a protein called eL18.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | Q | 187 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3149 | 946 | 1634 | 315 | 250 | 4 | | |

- Molecule 52 is a protein called eL28.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | r | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2045 | 616 | 1051 | 205 | 167 | 6 | | |

- Molecule 53 is a protein called Ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | QQ | 142 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2323 | 717 | 1195 | 213 | 195 | 3 | | |

- Molecule 54 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 54 | R | 180 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3172 | 933 | 1664 | 328 | 238 | 9 | | |

- Molecule 55 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 55 | s | 196 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3071 | 959 | 1564 | 263 | 276 | 9 | | |

- Molecule 56 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 56 | RR | 132 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2189 | 670 | 1121 | 199 | 195 | 4 | | |

- Molecule 57 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 57 | S | 176 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2970 | 930 | 1508 | 285 | 236 | 11 | | |

- Molecule 58 is a protein called uL12.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 58 | t | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2375 | 722 | 1215 | 218 | 217 | 3 | | |

- Molecule 59 is a protein called 40S ribosomal protein uS13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 59 | SS | 144 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2437 | 746 | 1247 | 241 | 202 | 1 | | |

- Molecule 60 is a protein called eL21.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 60 | T | 159 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2665 | 823 | 1367 | 252 | 217 | 6 | | |

- Molecule 61 is a protein called eS19.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 61 | TT | 141 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2229 | 688 | 1132 | 211 | 195 | 3 | | |

- Molecule 62 is a protein called L22.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 62 | U | 99 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1642 | 519 | 833 | 141 | 147 | 2 | | |

- Molecule 63 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 63 | UU | 100 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1657 | 498 | 862 | 152 | 141 | 4 | | |

- Molecule 64 is a protein called eL14.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 64 | V | 131 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2018 | 618 | 1039 | 184 | 172 | 5 | | |

- Molecule 65 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 65 | VV | 83 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1273 | 393 | 637 | 117 | 121 | 5 | | |

- Molecule 66 is a protein called 60S ribosomal protein L24-like protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 66 | W | 106 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1752 | 538 | 892 | 174 | 144 | 4 | | |

- Molecule 67 is a RNA chain called 28S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 67 | 5 | 3543 | Total | C | H | N | O | P | 0 | 0 |
| | | | 114361 | 33833 | 38389 | 13910 | 24686 | 3543 | | |

- Molecule 68 is a protein called Ribosomal protein S15a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 68 | WW | 129 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2114 | 659 | 1080 | 193 | 176 | 6 | | |

- Molecule 69 is a protein called uL23.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 69 | X | 118 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2007 | 618 | 1040 | 181 | 167 | 1 | | |

- Molecule 70 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 70 | 7 | 120 | Total | C | H | N | O | P | 0 | 0 |
| | | | 3854 | 1141 | 1296 | 456 | 842 | 119 | | |

- Molecule 71 is a protein called 40S ribosomal protein uS12.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 71 | XX | 141 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2263 | 693 | 1165 | 219 | 183 | 3 | | |

- Molecule 72 is a protein called Ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 72 | Y | 134 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2320 | 700 | 1205 | 226 | 186 | 3 | | |

- Molecule 73 is a RNA chain called 5.8S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 73 | 8 | 151 | Total | C | H | N | O | P | 0 | 0 |
| | | | 4837 | 1432 | 1629 | 564 | 1062 | 150 | | |

- Molecule 74 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 74 | YY | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2094 | 640 | 1083 | 198 | 168 | 5 | | |

- Molecule 75 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 75 | Z | 135 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2289 | 714 | 1182 | 208 | 182 | 3 | | |

- Molecule 76 is a RNA chain called 18S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 76 | 9 | 1698 | Total | C | H | N | O | P | 0 | 0 |
| | | | 54557 | 16180 | 18308 | 6508 | 11864 | 1697 | | |

- Molecule 77 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 77 | ZZ | 75 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1254 | 382 | 656 | 111 | 104 | 1 | | |

- Molecule 78 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 78 | a | 147 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2372 | 734 | 1210 | 239 | 185 | 4 | | |

- Molecule 79 is a protein called 40S_SA_C domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 79 | AA | 217 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3418 | 1086 | 1708 | 300 | 316 | 8 | | |

- Molecule 80 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 80 | aa | 101 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1678 | 507 | 864 | 170 | 132 | 5 | | |

- Molecule 81 is a protein called uL3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 81 | B | 394 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6482 | 2020 | 3310 | 597 | 542 | 13 | | |

- Molecule 82 is a protein called eL30.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 82 | c | 98 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1555 | 481 | 794 | 134 | 140 | 6 | | |

- Molecule 83 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 83 | CC | 221 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3522 | 1111 | 1806 | 295 | 301 | 9 | | |

- Molecule 84 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 84 | cc | 62 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1002 | 297 | 514 | 97 | 92 | 2 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| cc | 5 | HIS | ARG | conflict | UNP G1TIB4 |

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 85 | dd | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | ff | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | g | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | j | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | m | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | o | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | p | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | aa | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

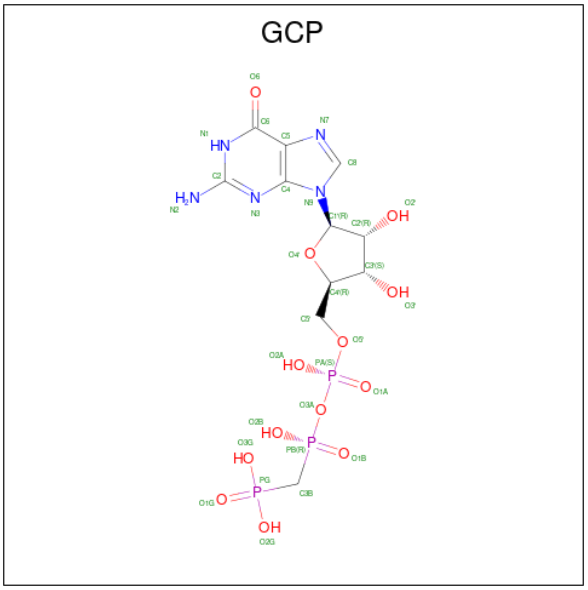
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 86 | hh | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 86 | j | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 86 | jj | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 86 | o | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 86 | P | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 86 | V | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

*Continued on next page...*

*Continued from previous page...*

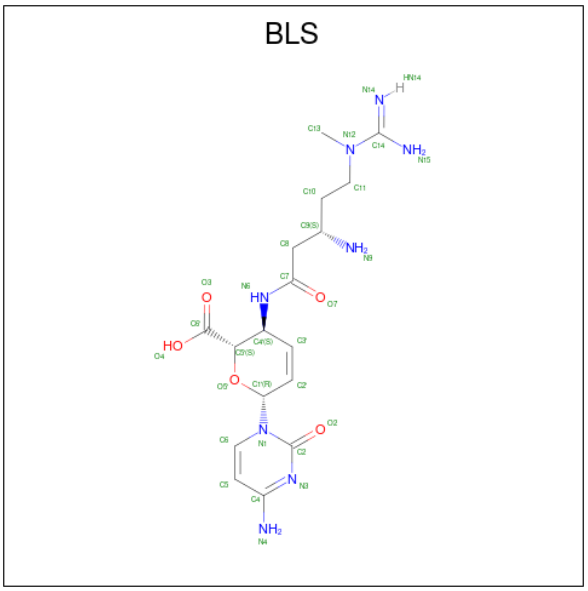
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 86 | 5 | 189 | Total Mg<br>189 189 | 0 |
| 86 | 7 | 4 | Total Mg<br>4 4 | 0 |
| 86 | 8 | 10 | Total Mg<br>10 10 | 0 |
| 86 | 9 | 70 | Total Mg<br>70 70 | 0 |
| 86 | a | 1 | Total Mg<br>1 1 | 0 |

- Molecule 87 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 87 | jj | 1 | Total C H N O P<br>46 11 14 5 13 3 | 0 |

- Molecule 88 is BLASTICIDIN S (three-letter code: BLS) (formula: $C_{17}H_{26}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



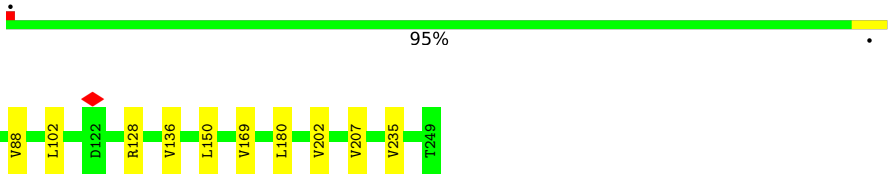

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 88 | 5 | 1 | Total | C | H | N | O | 0 |
| | | | 55 | 17 | 25 | 8 | 5 | |

# 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.

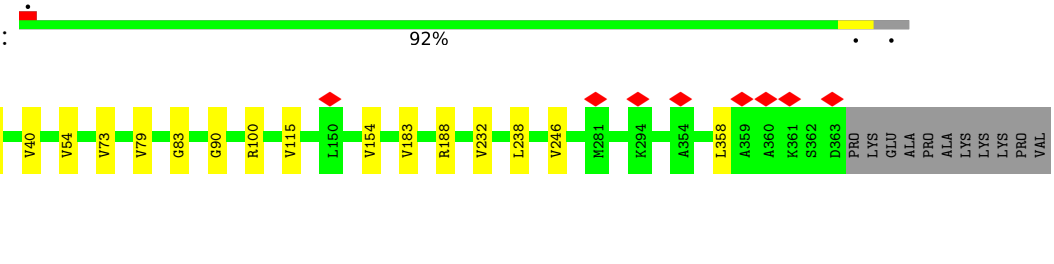
• Molecule 1: 60S ribosomal protein L8

Chain A:



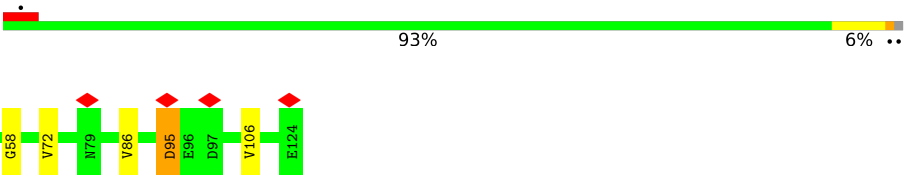

• Molecule 2: uL4

Chain C:



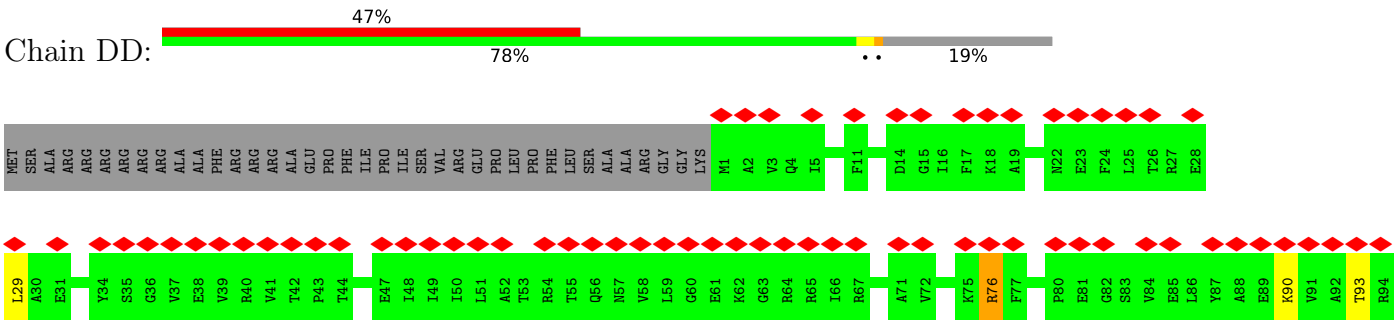

• Molecule 3: eL31

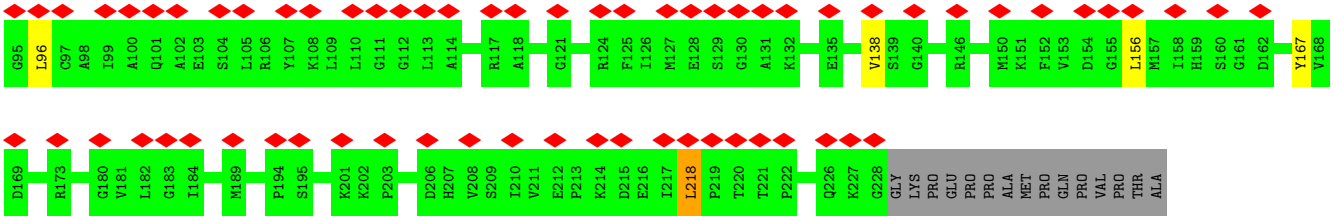
Chain d:



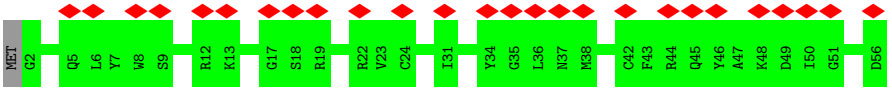

• Molecule 4: 40S ribosomal protein S3

Chain DD:

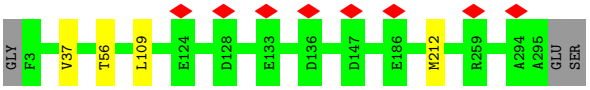




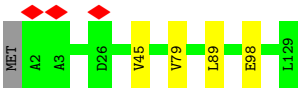

• Molecule 5: S29

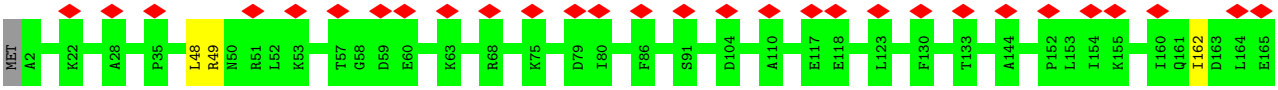

• Molecule 6: 60S ribosomal protein L5

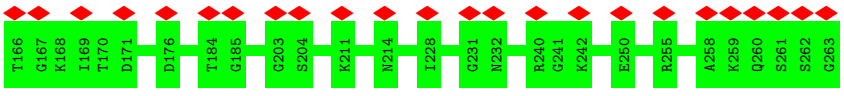




• Molecule 7: Ribosomal protein L32

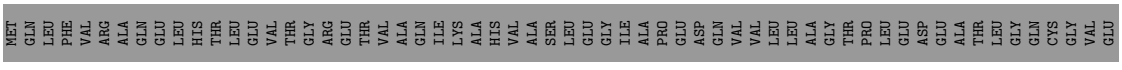



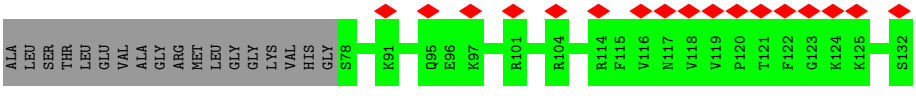

• Molecule 8: 40S ribosomal protein S4

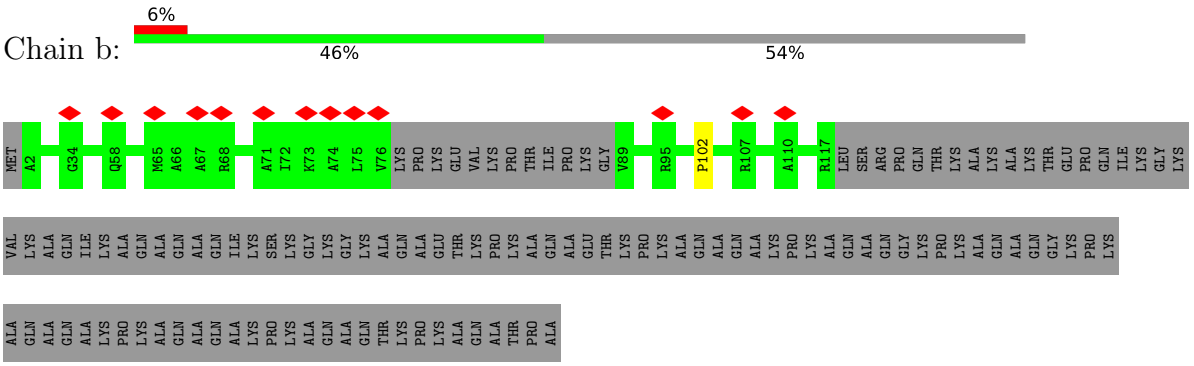

• Molecule 9: 40S ribosomal protein S30

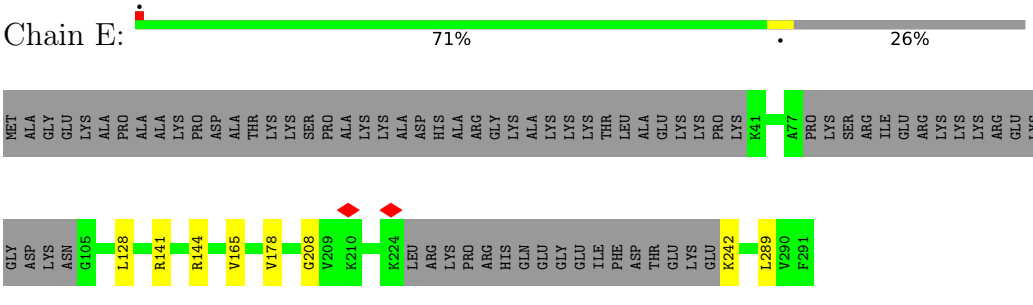
• Molecule 10: eL29

Chain b:



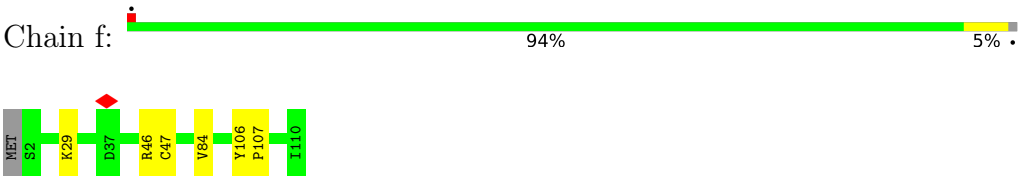

• Molecule 11: 60S ribosomal protein L6

Chain E:



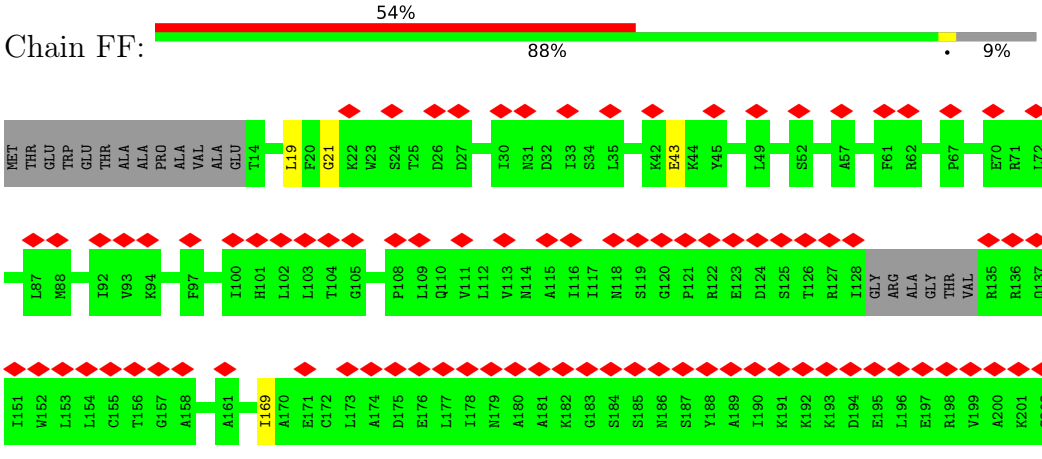

• Molecule 12: eL33

Chain f:



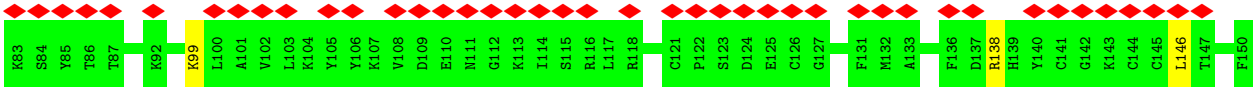

• Molecule 13: Ribosomal protein S5

Chain FF:



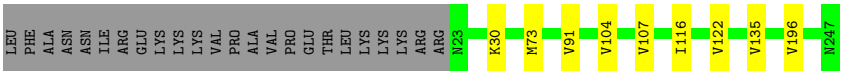

• Molecule 14: 40S ribosomal protein S27a

Chain ff:



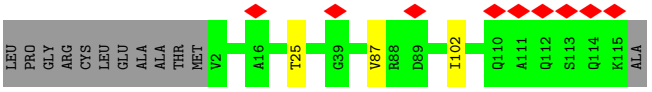

• Molecule 15: uL30

Chain F:

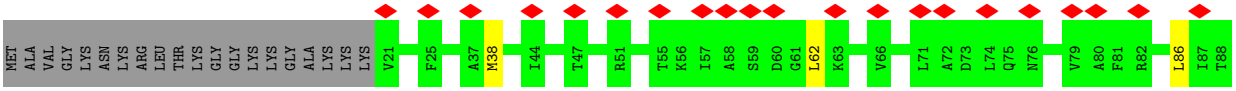

• Molecule 16: 60S ribosomal protein L34

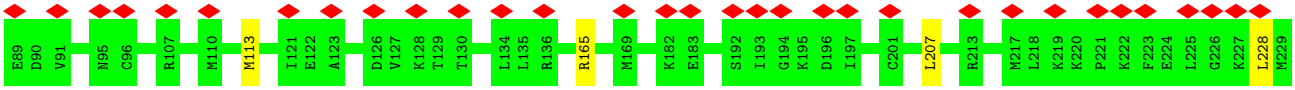
Chain g:

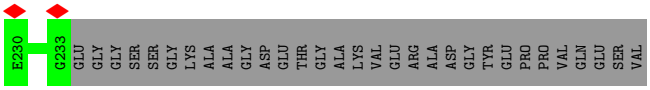




• Molecule 17: 40S ribosomal protein S3a

Chain BB:

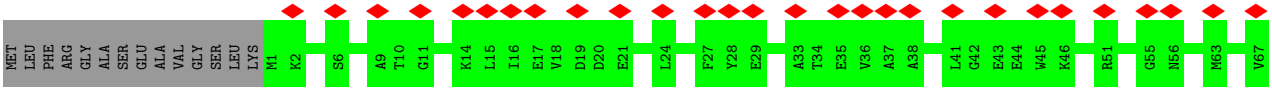



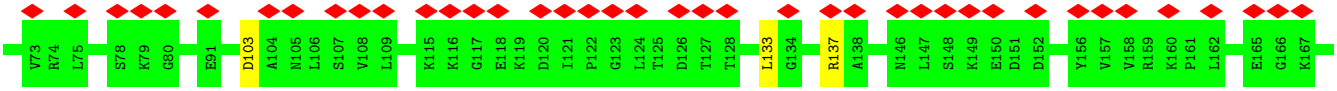



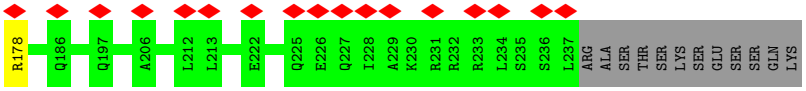




• Molecule 18: 40S ribosomal protein S6

Chain GG:

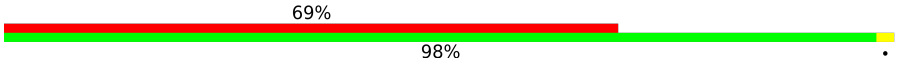



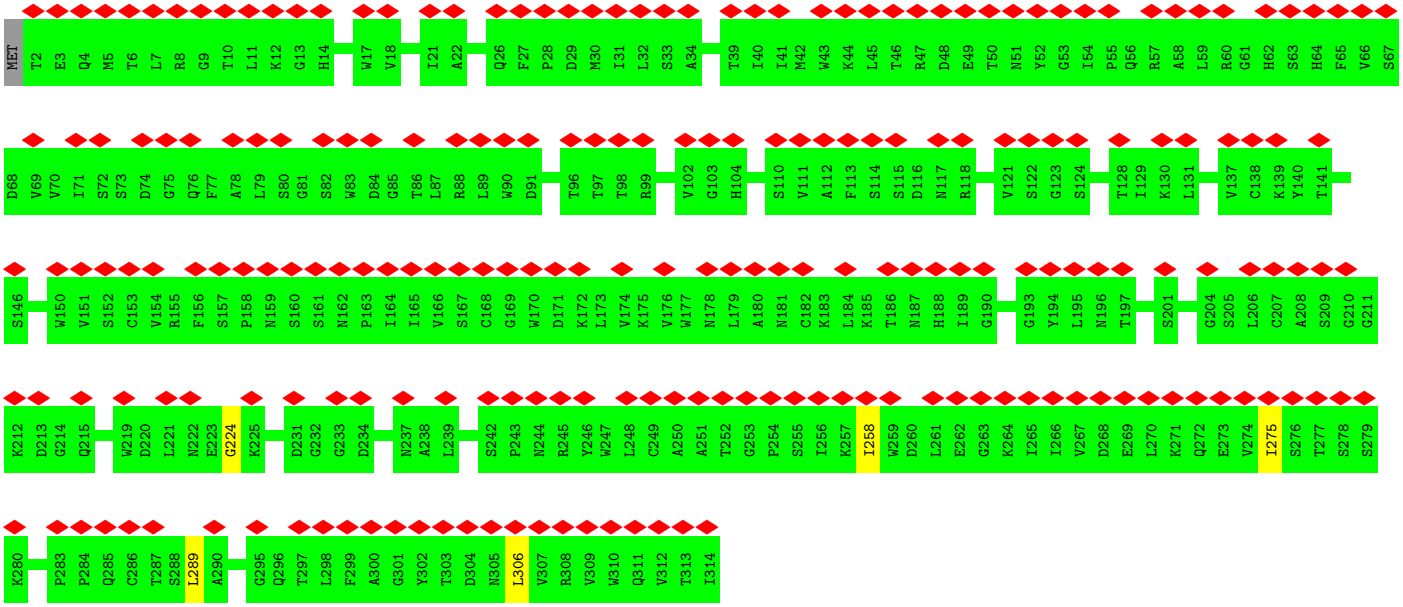




• Molecule 19: Epididymis tissue sperm binding protein Li 3a

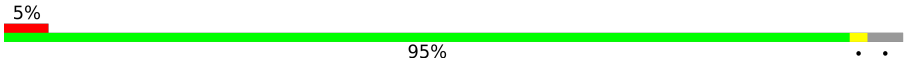
Chain gg:

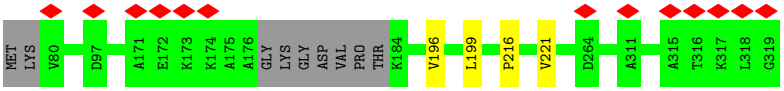



• Molecule 20: L7a

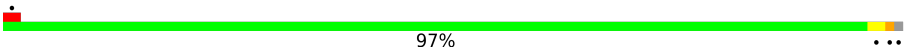
Chain G:

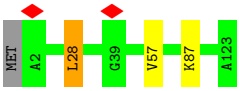



• Molecule 21: uL29

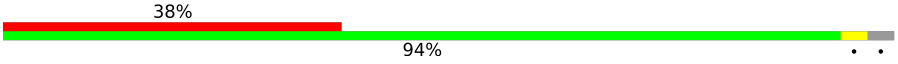
Chain h:

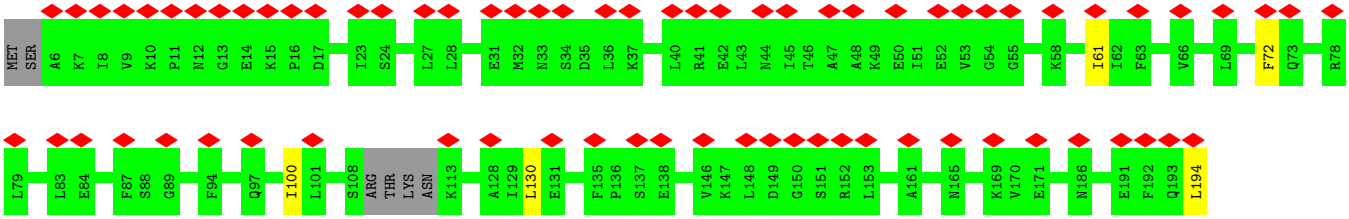



• Molecule 22: S7

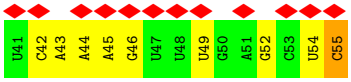
Chain HH:



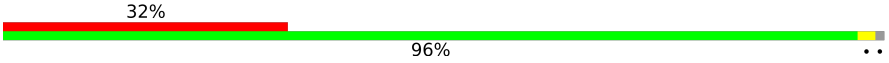

• Molecule 23: mRNA

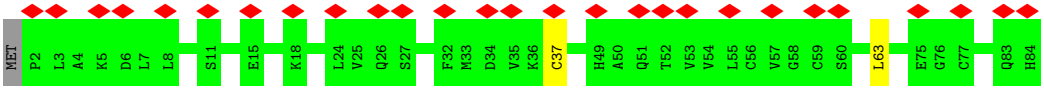
Chain hh:




• Molecule 24: 40S ribosomal protein S27

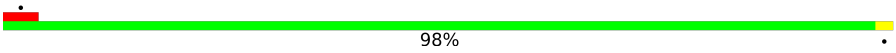
Chain bb:

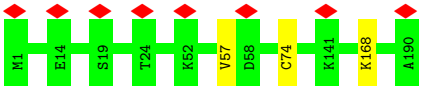



• Molecule 25: L9

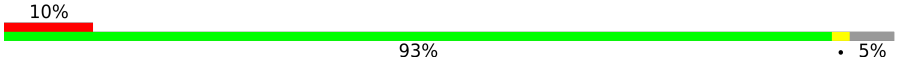
Chain H:

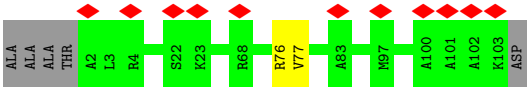



• Molecule 26: 60S ribosomal protein L36

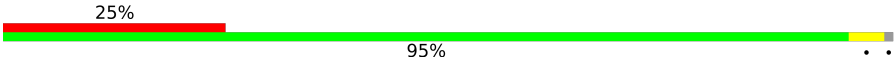
Chain i:

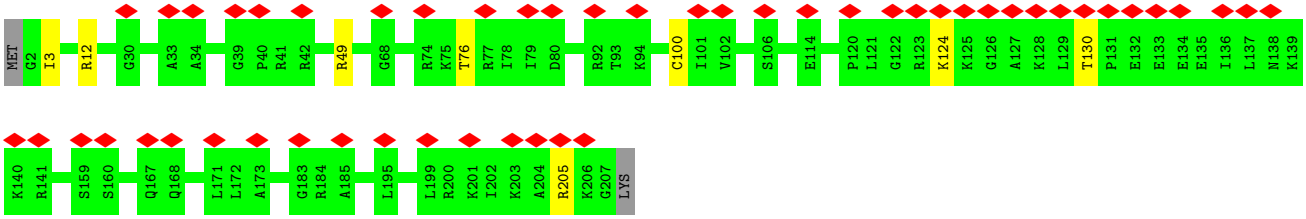



• Molecule 27: 40S ribosomal protein S8

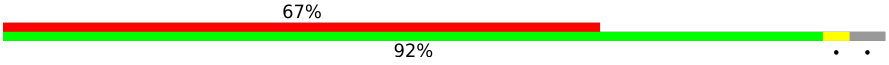
Chain II:

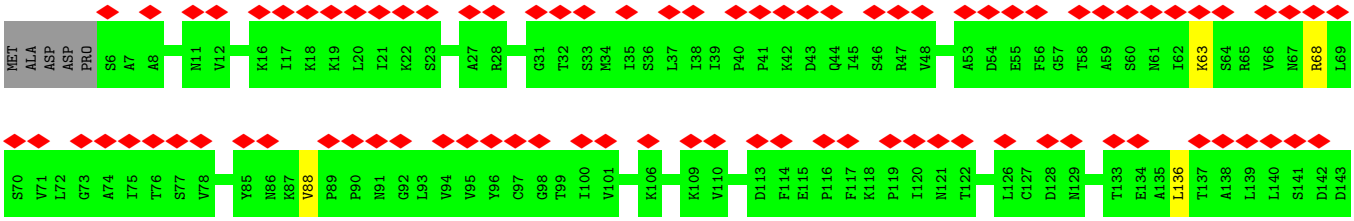


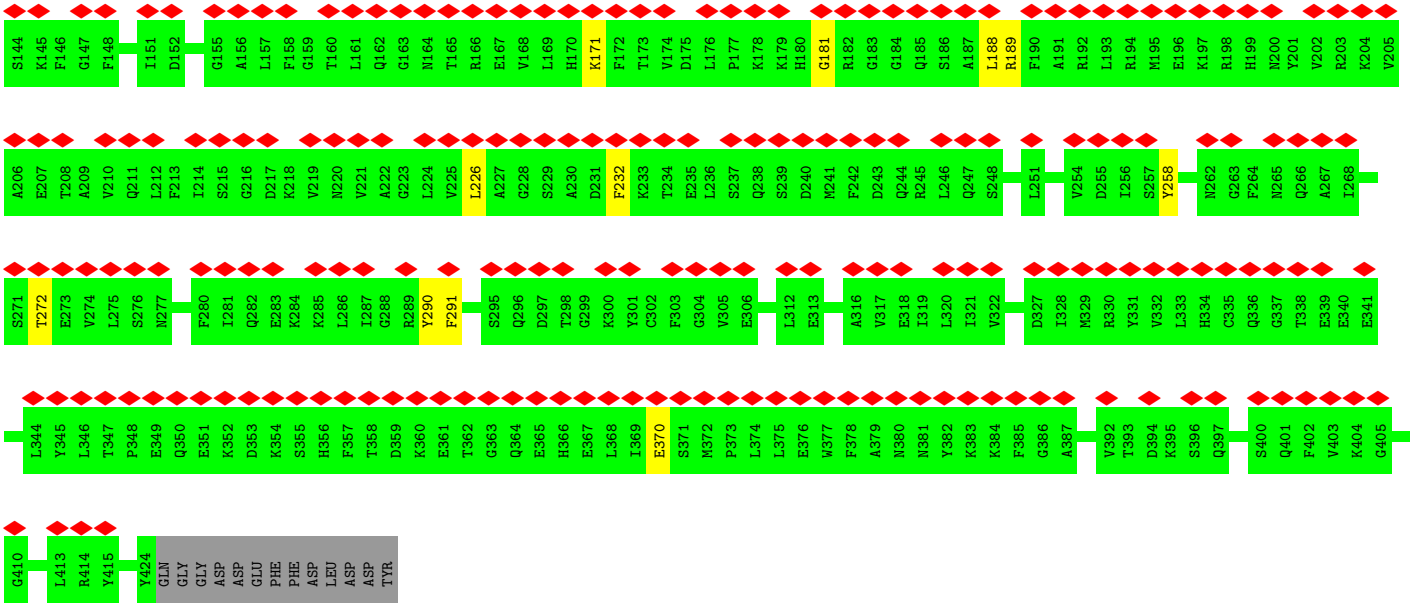




• Molecule 28: Eukaryotic peptide chain release factor subunit 1

Chain ii:

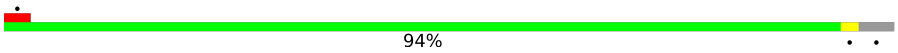


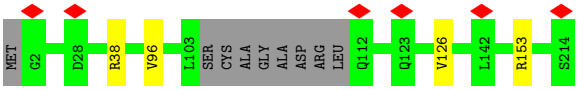






• Molecule 29: 60S ribosomal protein L10

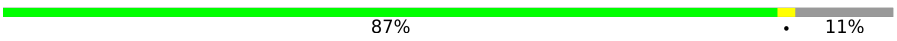
Chain I:

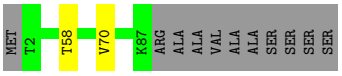



• Molecule 30: Ribosomal protein L37

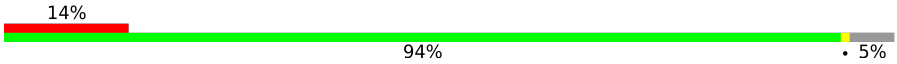
Chain j:

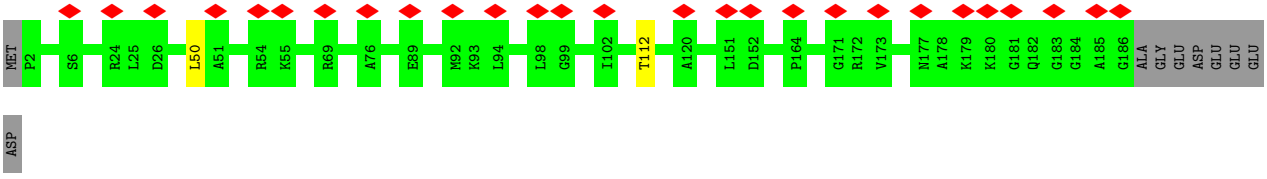



• Molecule 31: 40S ribosomal protein S9

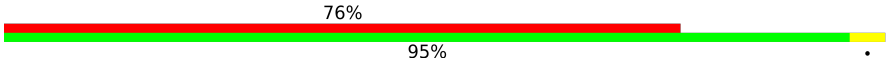
Chain JJ:

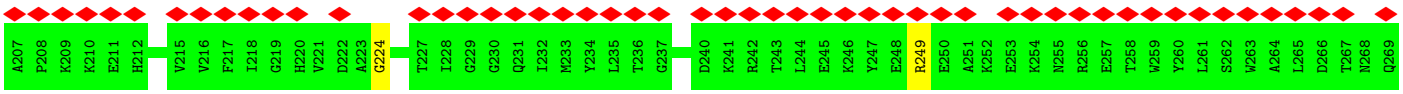


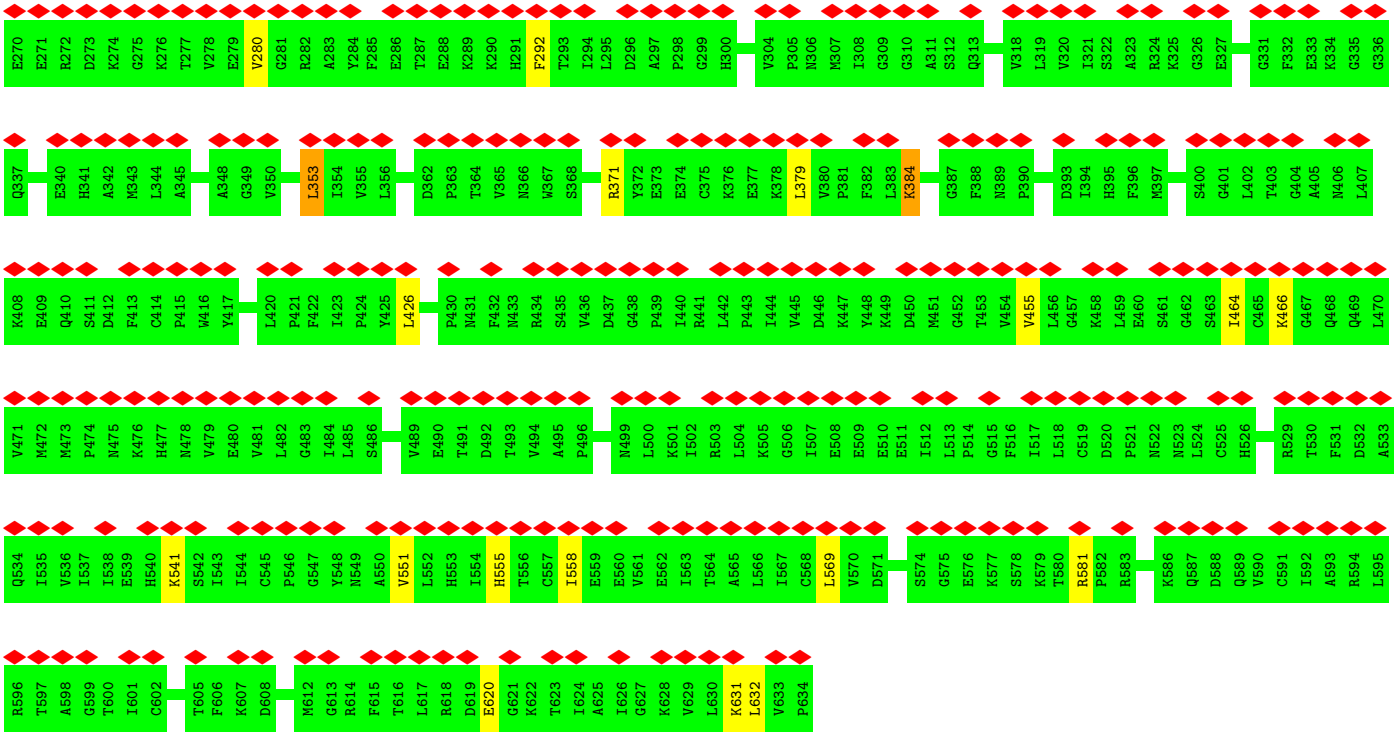




• Molecule 32: eRF3a

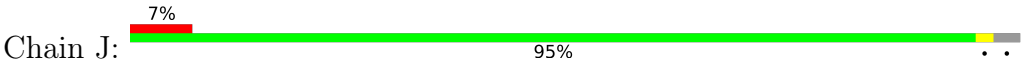
Chain jj:

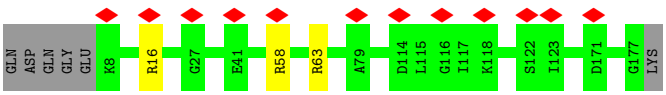


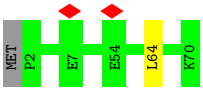



• Molecule 33: 60S ribosomal protein L11

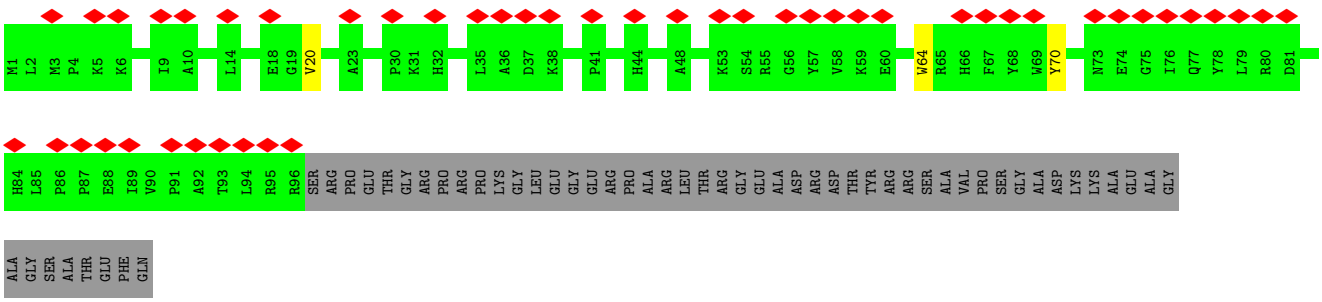



• Molecule 34: L38

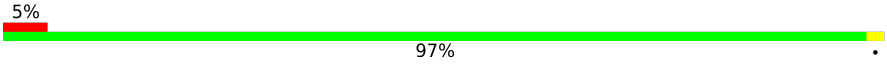



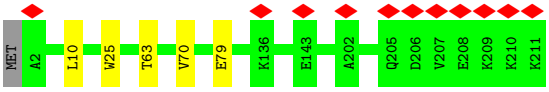

• Molecule 35: 40S ribosomal protein S10

• Molecule 36: 60S ribosomal protein L13

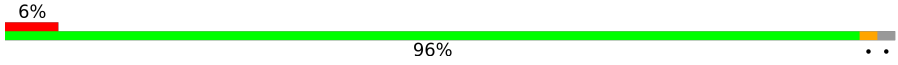
Chain L:

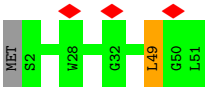



• Molecule 37: eL39

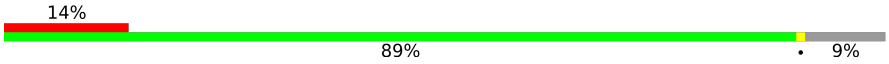
Chain l:

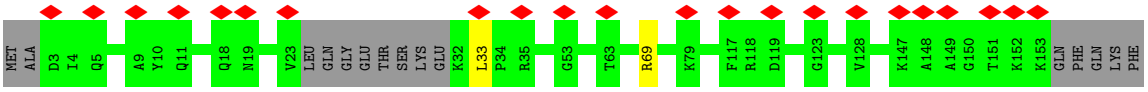



• Molecule 38: 40S ribosomal protein S11

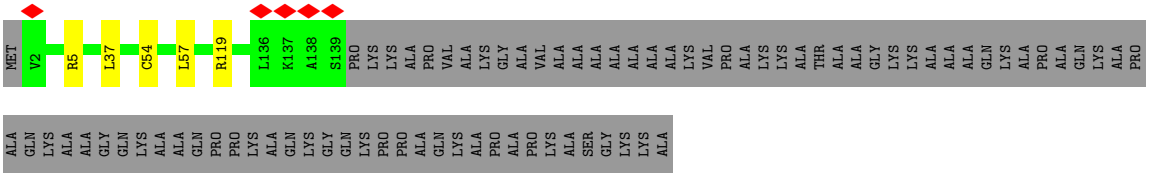
Chain LL:



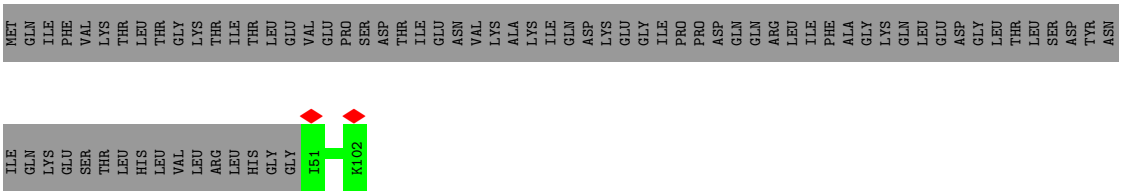

• Molecule 39: Ribosomal protein L14

Chain M:

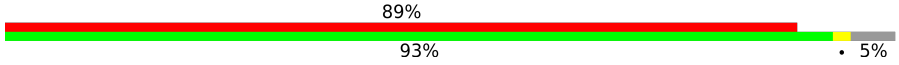

• Molecule 40: 60S RIBOSOMAL PROTEIN EL40

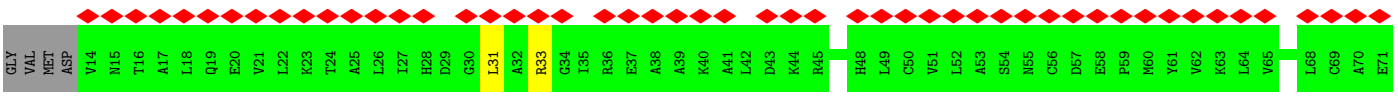
Chain m:

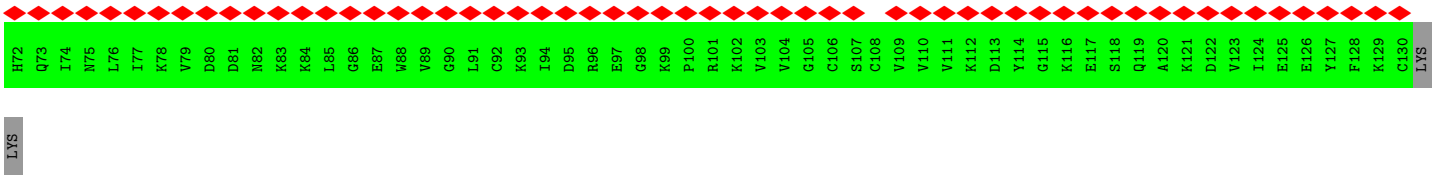




• Molecule 41: 40S ribosomal protein S12

Chain MM:

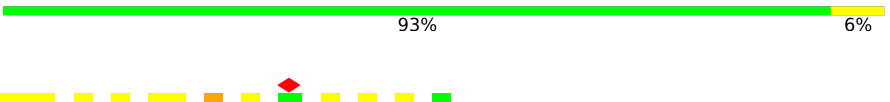




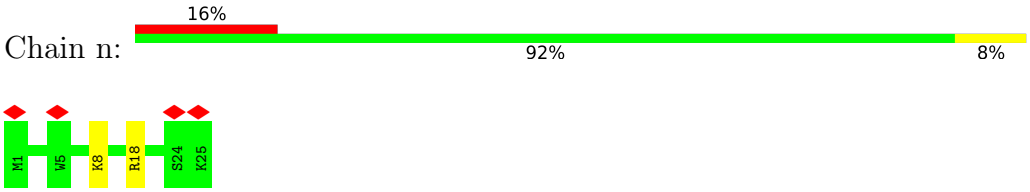

• Molecule 42: Ribosomal protein L15

Chain N:



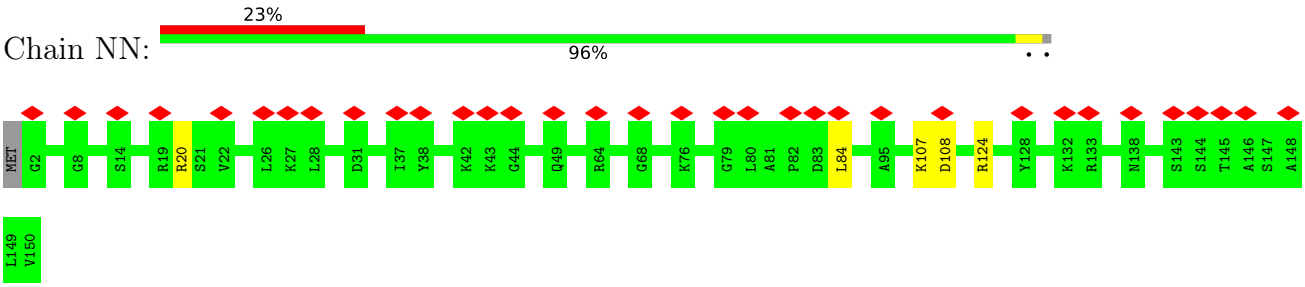

• Molecule 43: 60s ribosomal protein l41

Chain n:



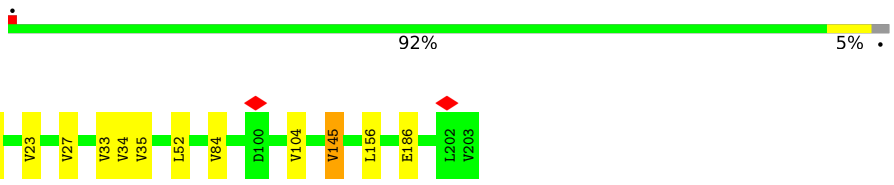

• Molecule 44: ribosomal protein uS15

Chain NN:



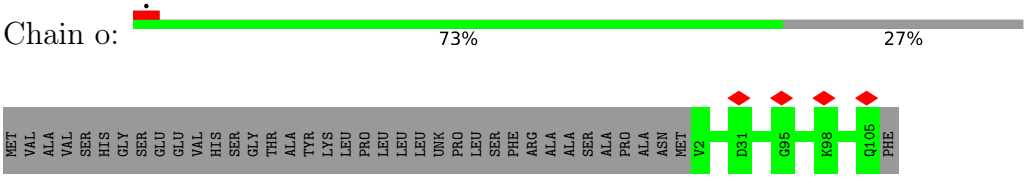

• Molecule 45: 60S RIBOSOMAL PROTEIN UL13

Chain O:



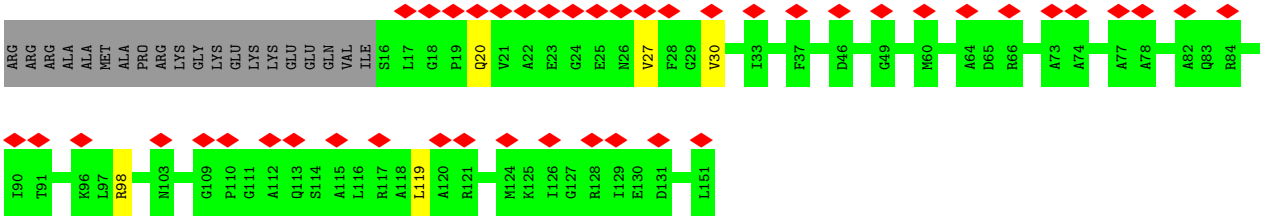

• Molecule 46: eL42

Chain o:

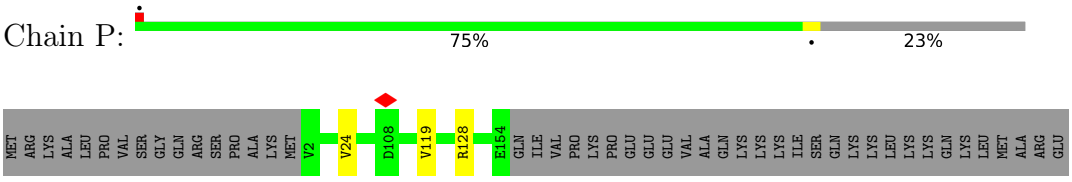



• Molecule 47: uS11

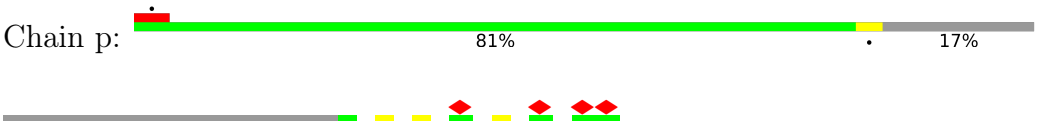
Chain OO:



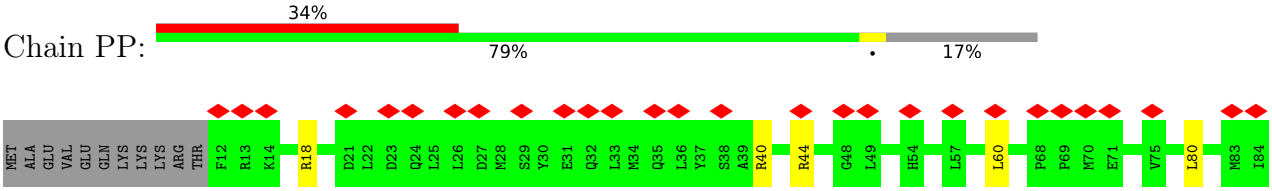

• Molecule 48: uL22



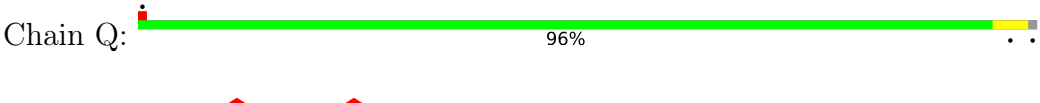

• Molecule 49: ribosomal protein eL43



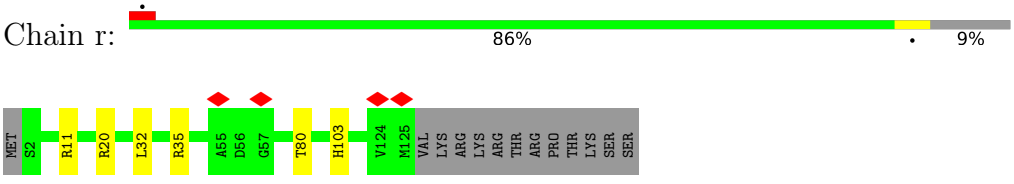

• Molecule 50: 40S ribosomal protein uS19




• Molecule 51: eL18

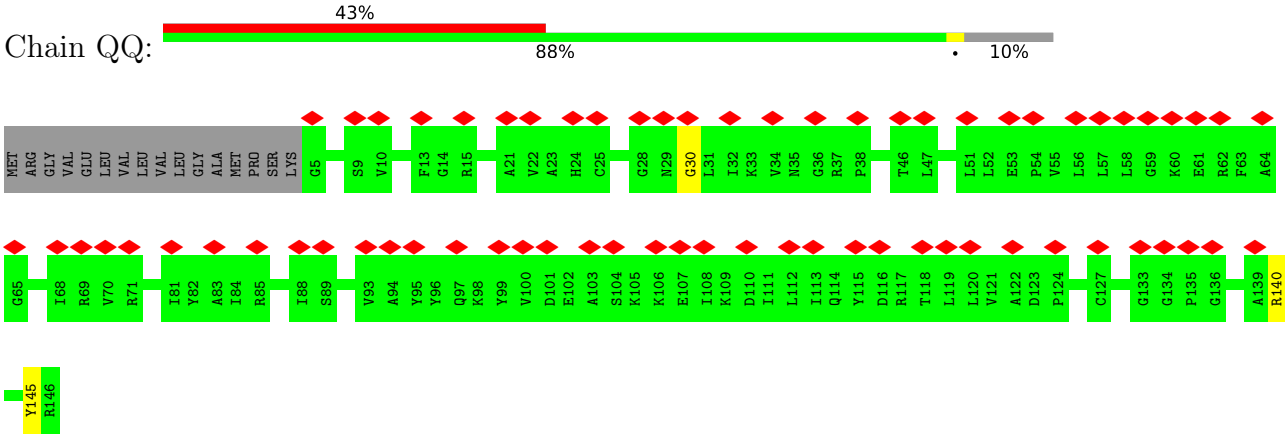



• Molecule 52: eL28



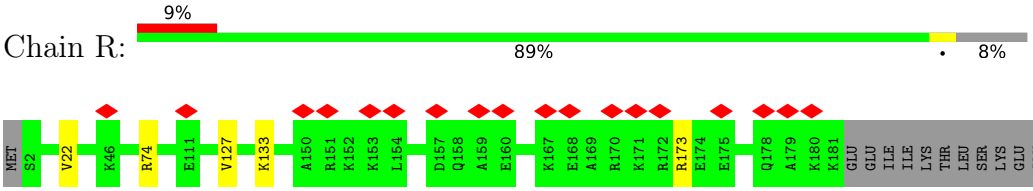

• Molecule 53: Ribosomal protein S16

Chain QQ:



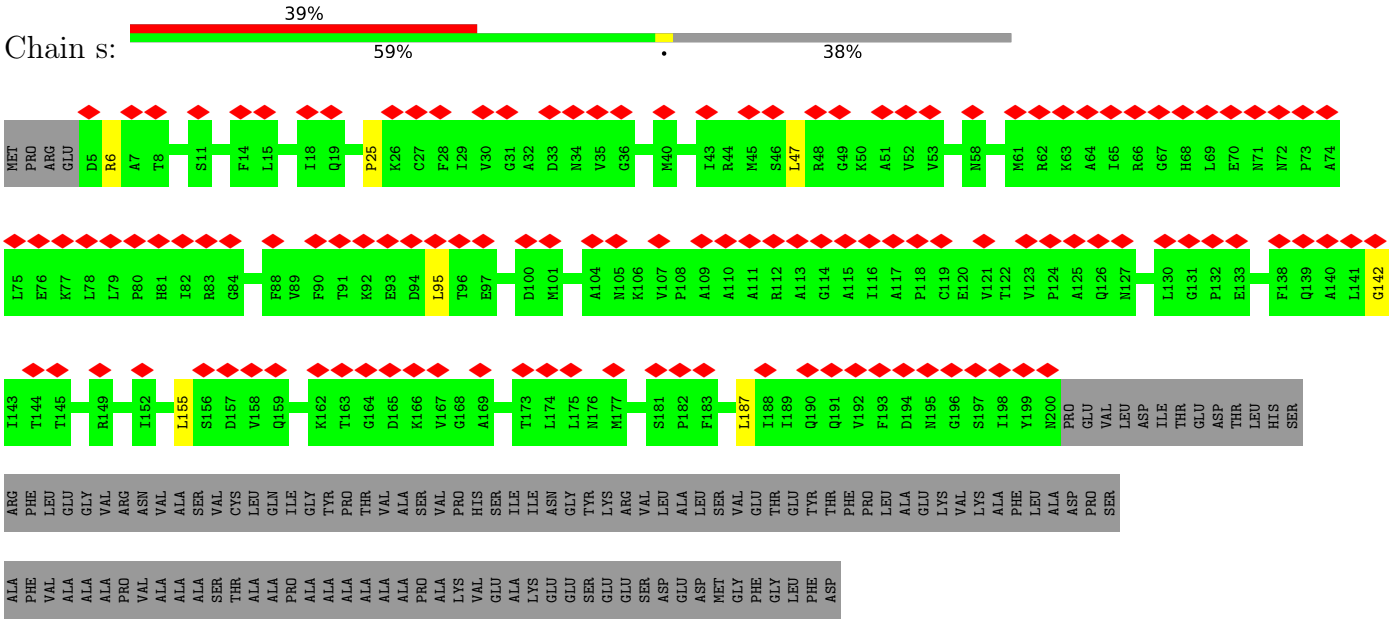

• Molecule 54: 60S ribosomal protein L19

Chain R:



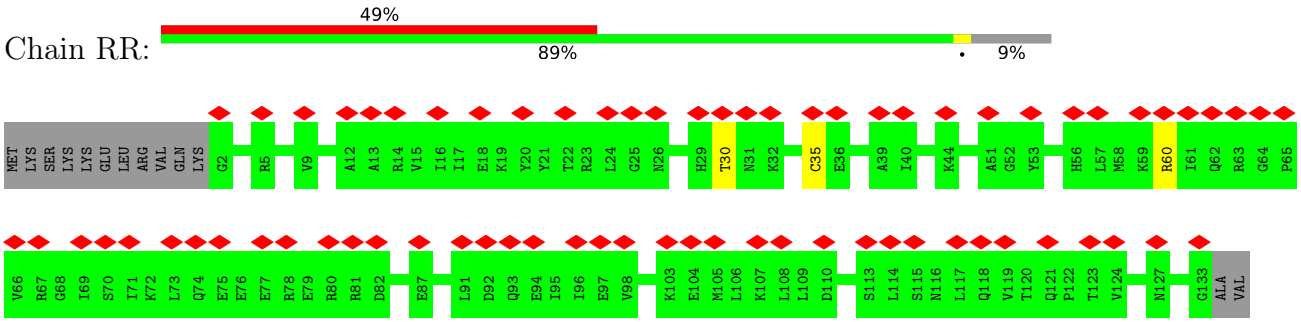

• Molecule 55: 60S acidic ribosomal protein P0

Chain s:



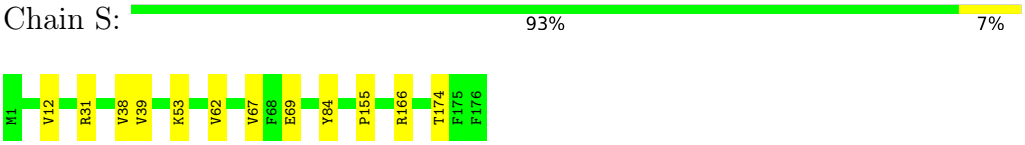

• Molecule 56: 40S ribosomal protein S17

Chain RR:



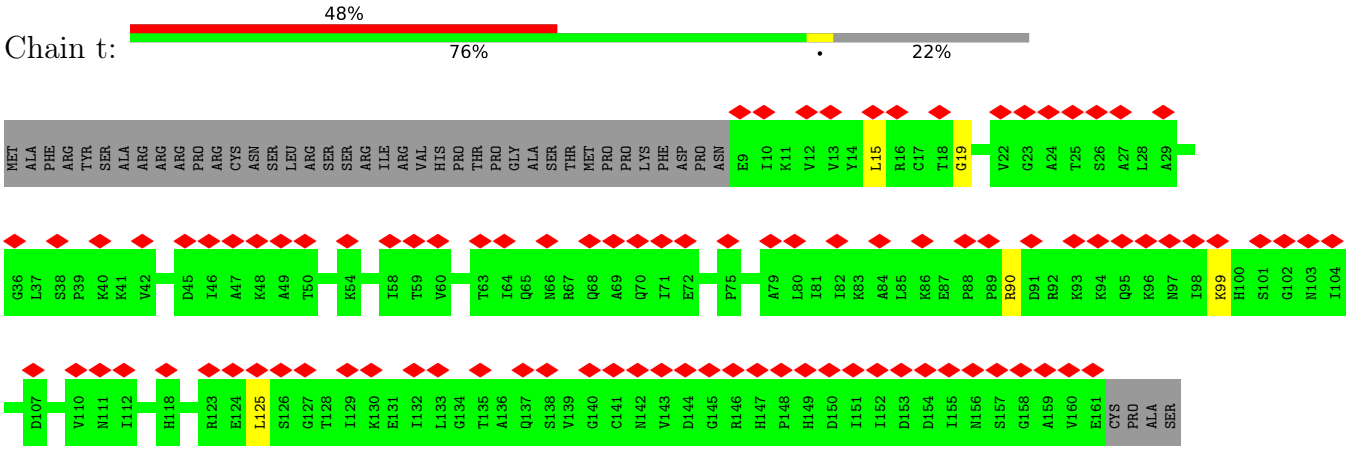
• Molecule 57: 60S ribosomal protein L18a

Chain S:



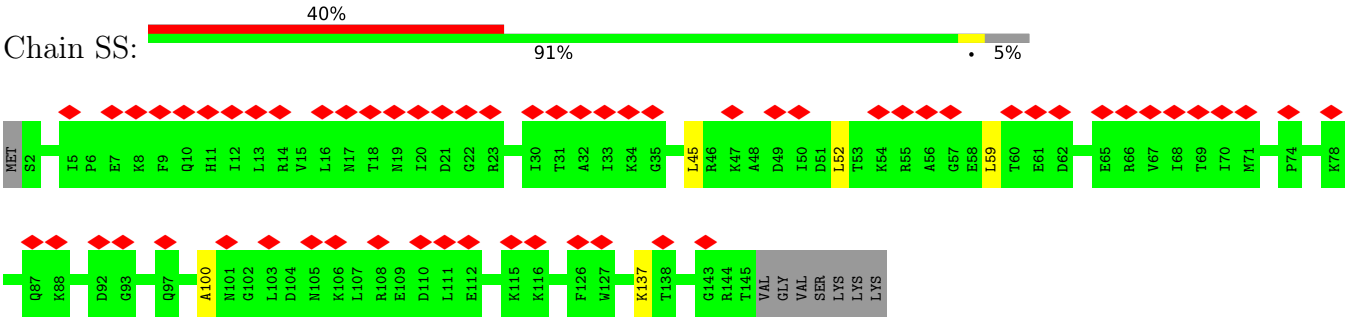

• Molecule 58: uL12

Chain t:



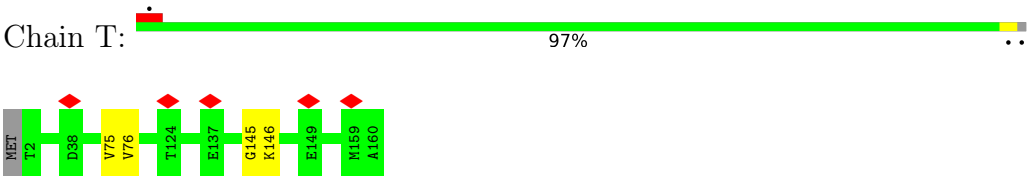

• Molecule 59: 40S ribosomal protein uS13

Chain SS:



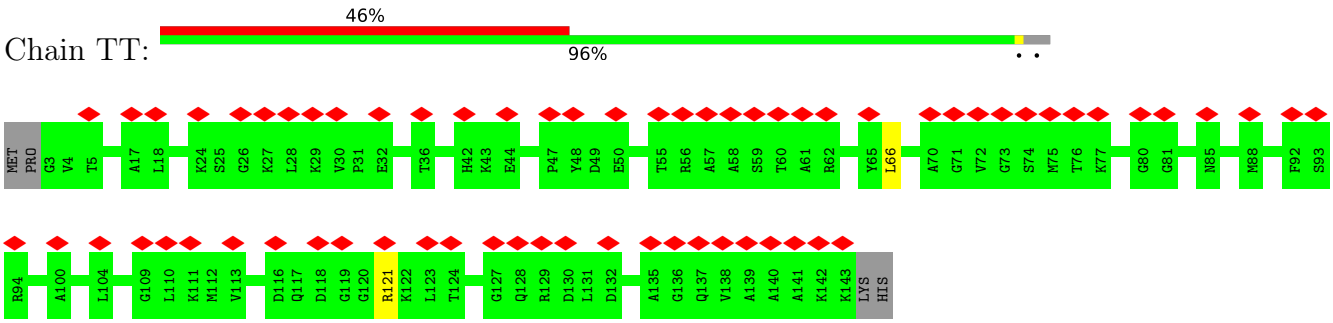

• Molecule 60: eL21

Chain T:



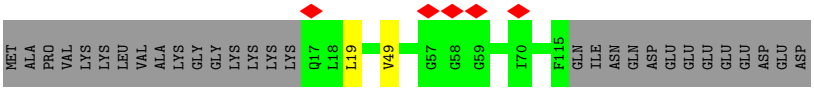

• Molecule 61: eS19

Chain TT:



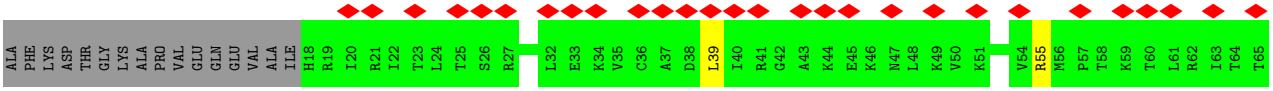
• Molecule 62: L22

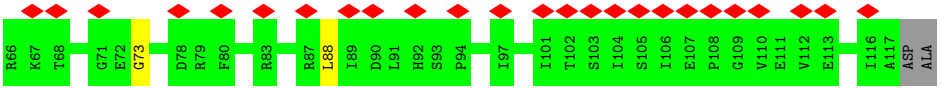
Chain U:


• Molecule 63: 40S ribosomal protein S20

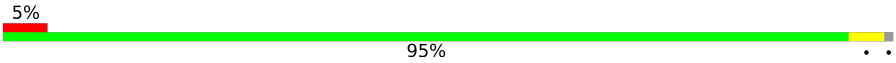
Chain UU:

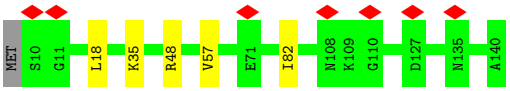




• Molecule 64: eL14

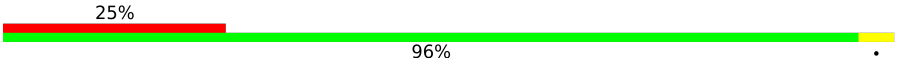
Chain V:

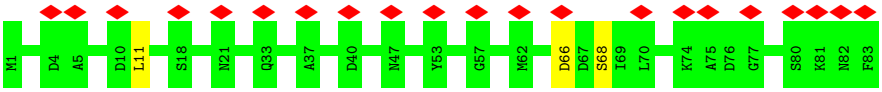



• Molecule 65: 40S ribosomal protein S21

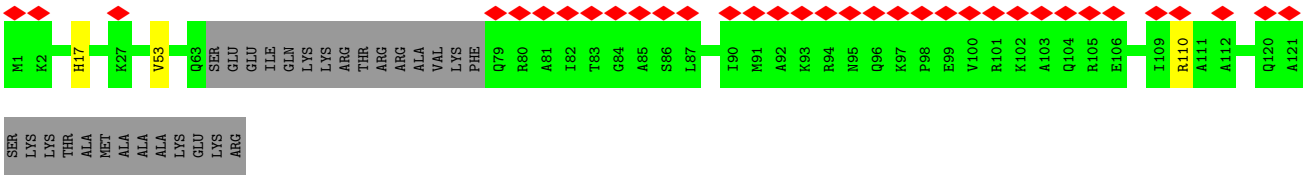
Chain VV:



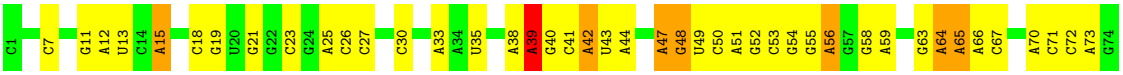

• Molecule 66: 60S ribosomal protein L24-like protein

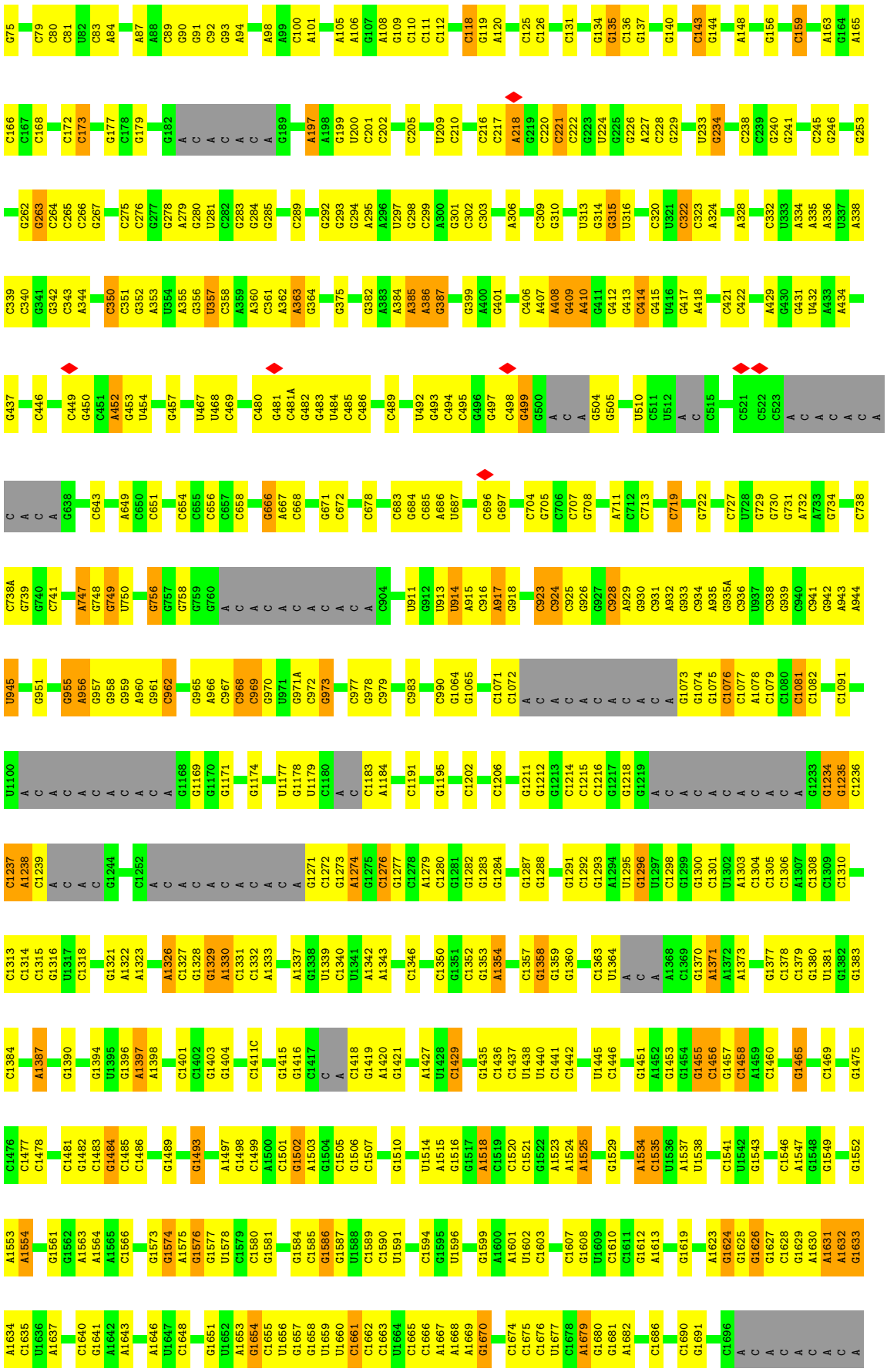
Chain W:


• Molecule 67: 28S Ribosomal RNA

Chain 5: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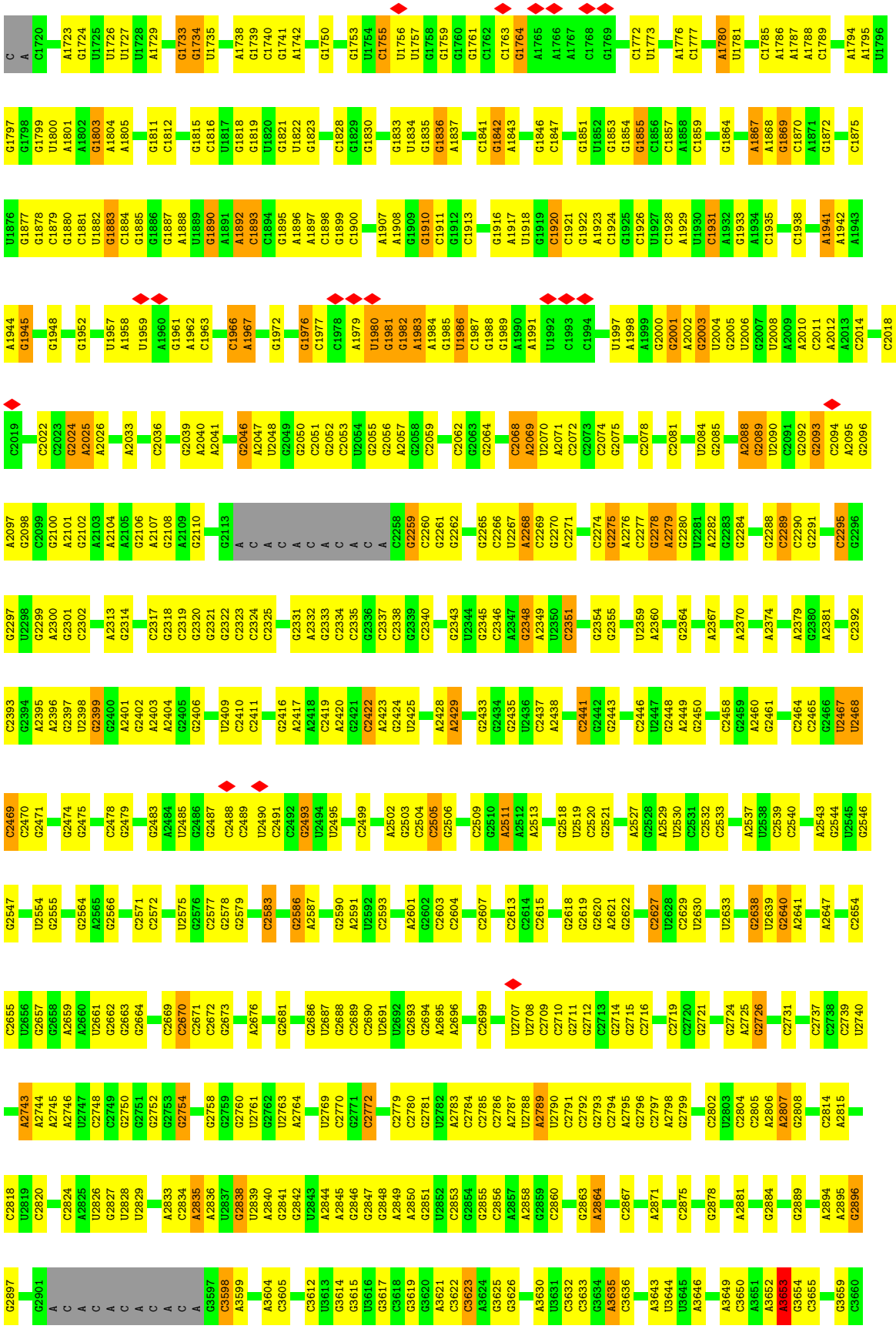
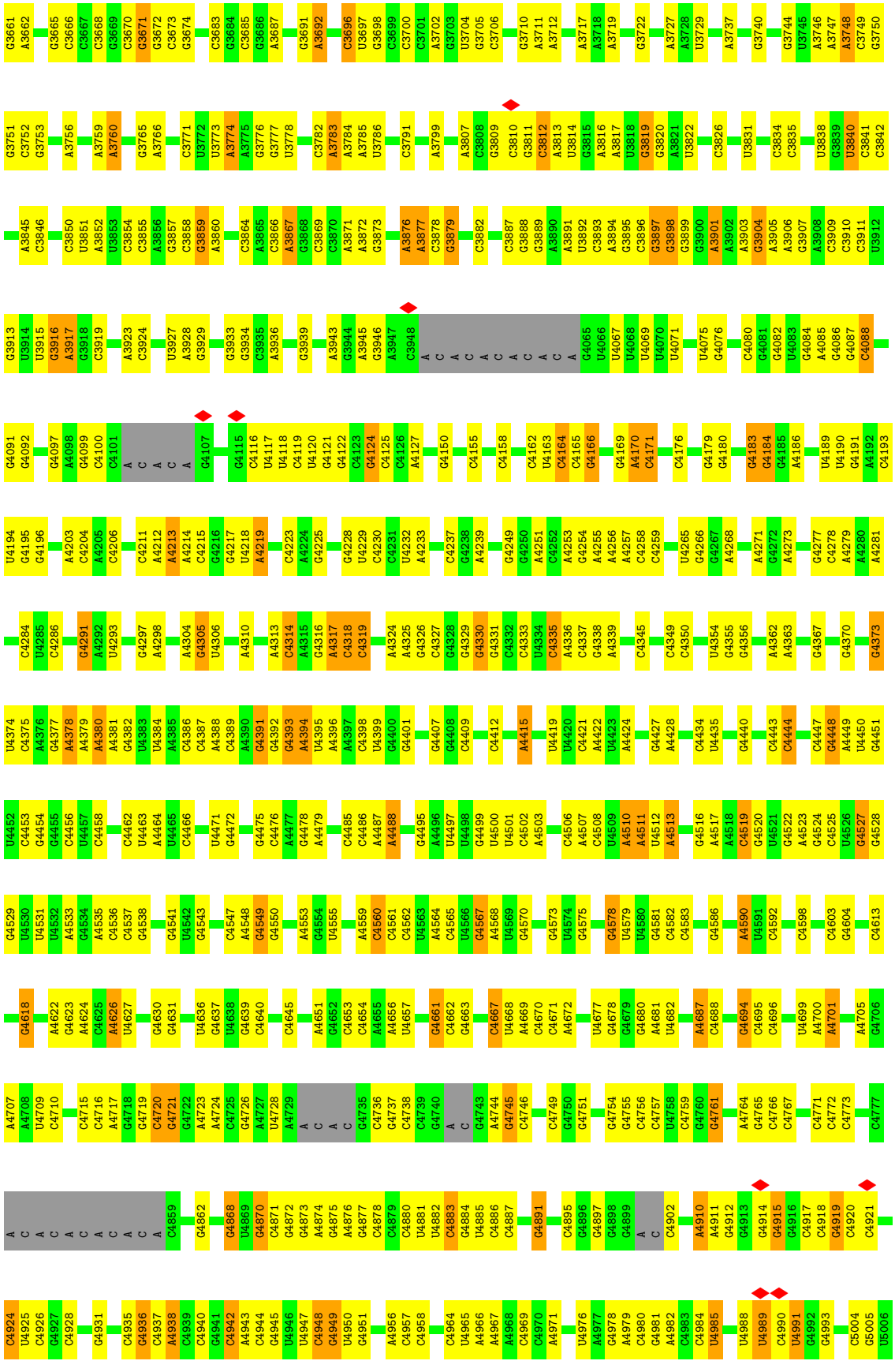
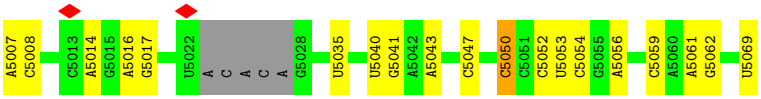
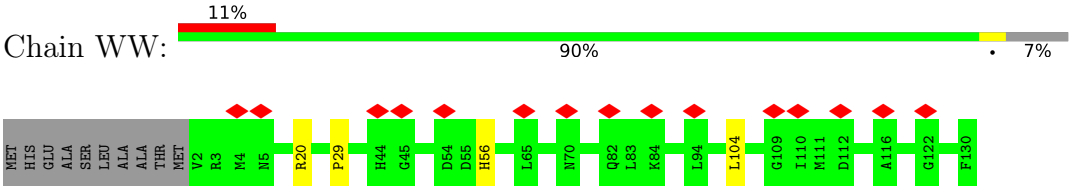
C166 C167 C168 C172 C173 G177 C178 G179 G182 A C C A C A A G189 A197 A198 G199 U200 C201 C202 C205 U209 C210 C216 C217 A218 G219 C220 C221 C222 G223 U224 G225 G226 A227 C228 G229 U233 G234 C238 C239 G240 G241 C245 G246 G253
G262 G263 C264 C265 C266 G267 C275 C276 G277 G278 A279 G280 U281 C282 G283 G284 G285 C289 G292 G293 G294 A295 A296 U297 G298 C299 A300 G301 C302 C303 A306 C309 G310 U313 G314 G315 U316 C320 U321 C322 C323 A324 A328 C332 U333 A334 A335 A336 U337 A338
C339 C340 G341 G342 C343 A344 C350 C351 G352 A353 U354 A355 G356 U357 C358 A359 A360 C361 A362 A363 G364 G375 G382 A383 A384 A385 A386 G387 G399 A400 G401 C406 A407 A408 G409 A410 G411 G412 G413 C414 G415 U416 G417 A418 C421 C422 A429 G430 G431 U432 A433 A434
G437 C446 C449 G450 C451 A452 G453 U454 G457 U467 U468 C469 C480 G481 C481A G482 G483 U484 C485 C486 C489 U492 G493 C494 C495 G496 G497 C498 G499 G500 A C A G504 G505 U510 C511 U512 A C C515 C521 C522 C523 A C A C A
C G A C A G638 C643 A649 C650 C651 C654 C655 C656 C657 C658 G666 A667 C668 G671 C672 C678 C683 G684 C685 A686 U687 C696 G697 C704 G705 C706 C707 G708 A711 C712 C713 C719 G722 C727 U728 G729 G730 G731 A732 A733 G734 C738
C738A G739 G740 C741 A747 G748 G749 U750 G756 G757 G758 G759 G760 A C C A C A C904 U911 G912 U913 U914 A915 C916 A917 G918 C923 C924 C925 G926 G927 C928 A929 G930 C931 A932 G933 C934 A935 G935A C936 U937 C938 G939 C940 C941 G942 A943 A944
U945 G951 G955 A956 G957 G958 G959 A960 G961 C962 G965 A966 C967 C968 C969 G970 U971 G971A C972 G973 C977 G978 C979 C983 C990 G1064 G1065 C1071 C1072 A C A C A C A G1073 G1074 G1075 C1076 C1077 A1078 C1079 C1080 C1081 C1082 C1091
U1100 A C A C A C A C G1168 G1169 G1170 G1171 G1174 U1177 G1178 U1179 C1180 A C C1183 A1184 C1191 G1195 C1202 C1206 G1211 G1212 G1213 C1214 C1215 C1216 G1217 G1218 G1219 A C A C A C A C G1233 G1234 G1235 C1236
C1237 A1238 C1239 A C A C A C A C G1244 C1252 A C A C A C A C G1271 C1272 G1273 A1274 G1275 C1276 G1277 C1278 A1279 C1280 G1281 C1282 G1283 G1284 G1287 G1288 G1291 C1292 G1293 A1294 U1295 G1296 U1297 C1298 G1299 G1300 C1301 U1302 A1303 C1304 C1305 C1306 A1307 C1308 C1309 C1310
C1313 C1314 C1315 G1316 U1317 C1318 G1321 A1322 A1323 A1326 C1327 G1328 G1329 A1330 C1331 C1332 A1333 A1337 G1338 U1339 C1340 U1341 A1342 A1343 C1346 C1350 G1351 C1352 G1353 A1354 C1357 G1358 G1359 G1360 C1363 U1364 A C A A1368 C1369 G1370 A1371 A1372 A1373 G1377 C1378 C1379 G1380 U1381 G1382 G1383
C1384 A1387 G1390 G1394 U1395 G1396 A1397 A1398 C1401 C1402 G1403 G1404 C1411C G1415 G1416 C1417 C A C1418 G1419 A1420 G1421 A1427 U1428 C1429 G1435 C1436 C1437 U1438 U1440 C1441 C1442 U1445 C1446 G1451 A1452 G1453 G1454 G1455 C1456 G1457 C1458 A1459 C1460 G1465 G1469 G1475
C1476 C1477 C1478 C1481 G1482 C1483 G1484 C1485 C1486 G1489 G1493 A1497 G1498 C1499 A1500 C1501 G1502 A1503 G1504 C1505 G1506 C1507 G1510 U1514 A1515 G1516 G1517 A1518 C1519 C1520 C1521 G1522 A1523 A1524 A1525 G1529 A1534 C1535 U1536 A1537 U1538 C1541 U1542 G1543 C1546 A1547 G1548 G1549 G1552
A1553 A1554 G1561 G1562 A1563 A1564 A1565 C1566 G1573 G1574 A1575 G1576 G1577 U1578 C1579 C1580 G1581 G1584 C1585 G1586 G1587 U1588 C1589 C1590 U1591 C1594 G1595 U1596 G1599 A1600 A1601 U1602 C1603 C1607 G1608 U1609 C1610 C1611 G1612 A1613 G1619 A1623 G1624 G1625 G1626 G1627 C1628 G1629 A1630 A1631 A1632 G1633
A1634 C1635 U1636 A1637 C1640 G1641 A1642 A1643 A1646 U1647 C1648 G1651 U1652 A1653 G1654 C1655 U1656 G1657 G1658 U1659 U1660 C1661 C1662 C1663 U1664 C1665 C1666 A1667 A1668 A1669 G1670 C1674 C1675 C1676 U1677 C1678 A1679 G1680 G1681 A1682 C1686 C1690 G1691 C1696 A C A C A C A



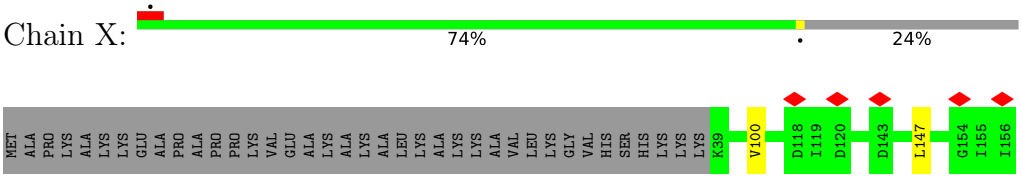




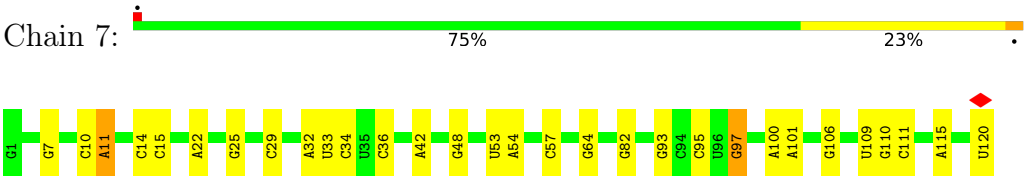

• Molecule 68: Ribosomal protein S15a



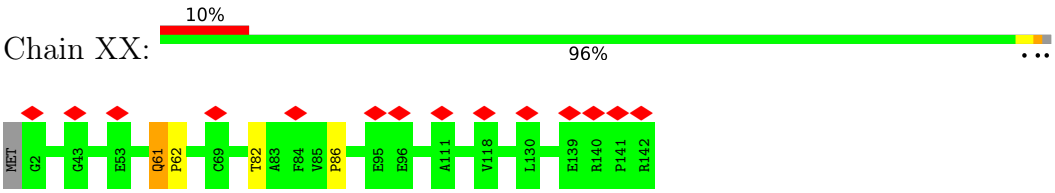

• Molecule 69: uL23



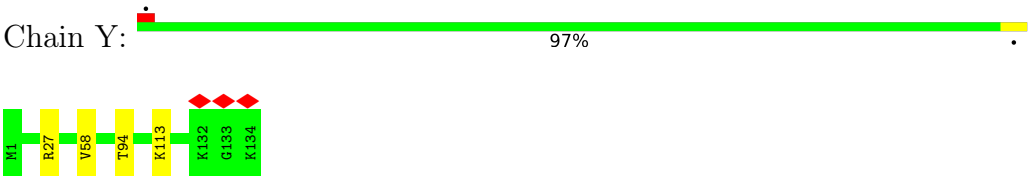

• Molecule 70: 5S Ribosomal RNA



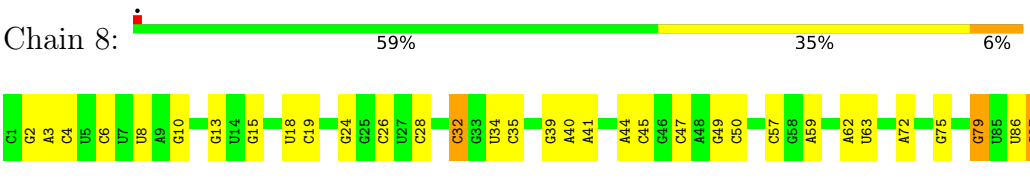

• Molecule 71: 40S ribosomal protein uS12




• Molecule 72: Ribosomal protein L26

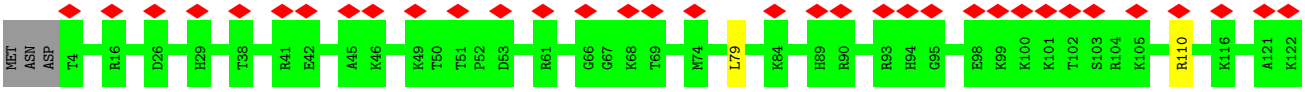


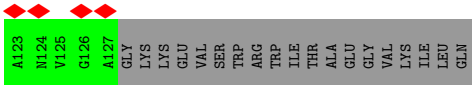

• Molecule 73: 5.8S Ribosomal RNA




• Molecule 74: 40S ribosomal protein S24

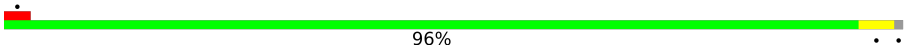
Chain YY:

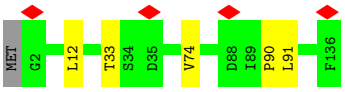




• Molecule 75: 60S ribosomal protein L27

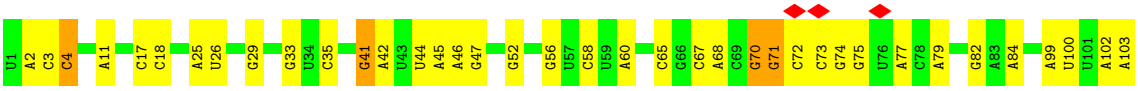
Chain Z:

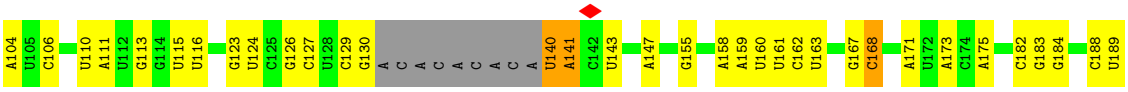


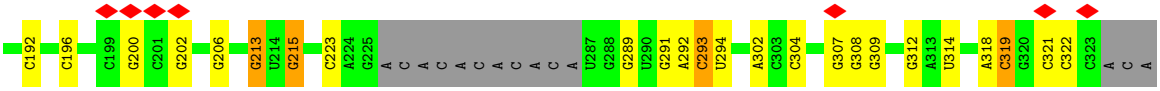



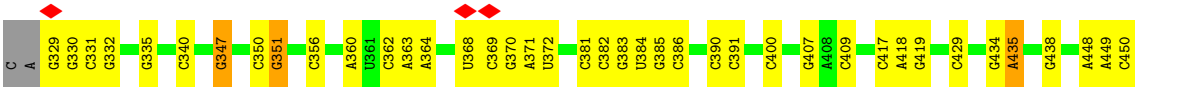

• Molecule 76: 18S Ribosomal RNA

Chain 9:

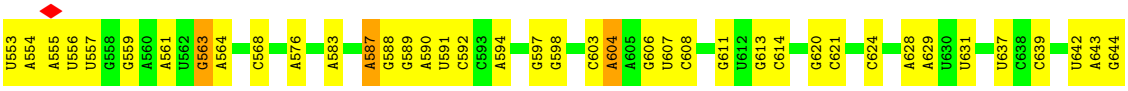



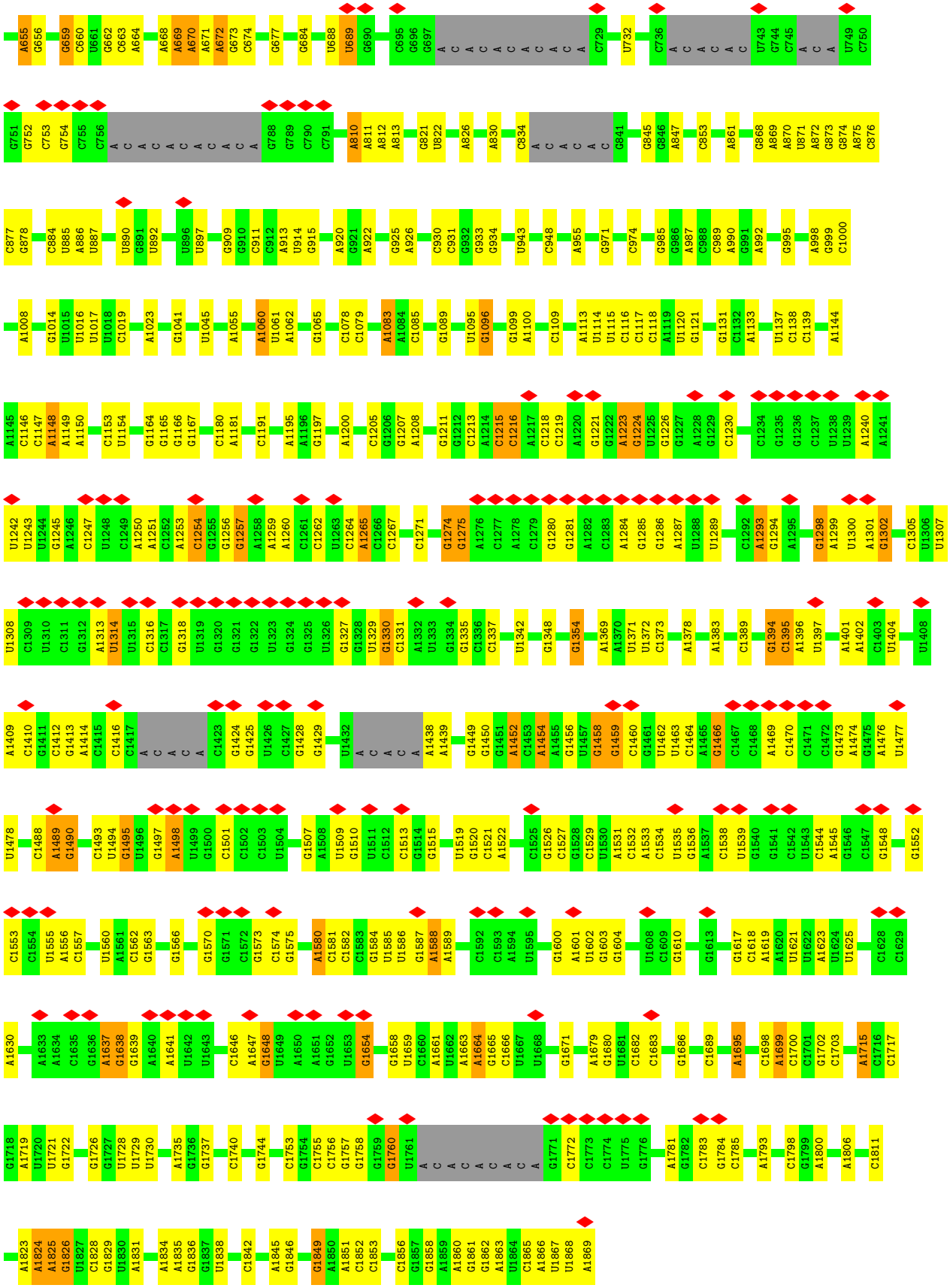



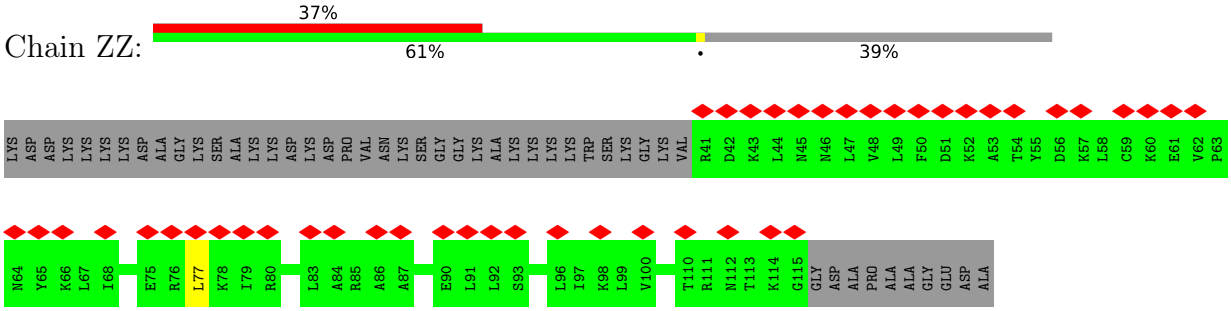






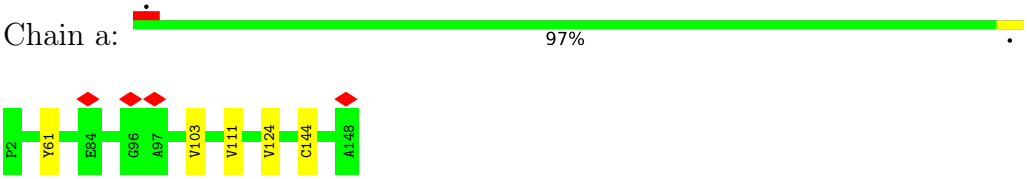
• Molecule 77: 40S ribosomal protein S25

Chain ZZ:



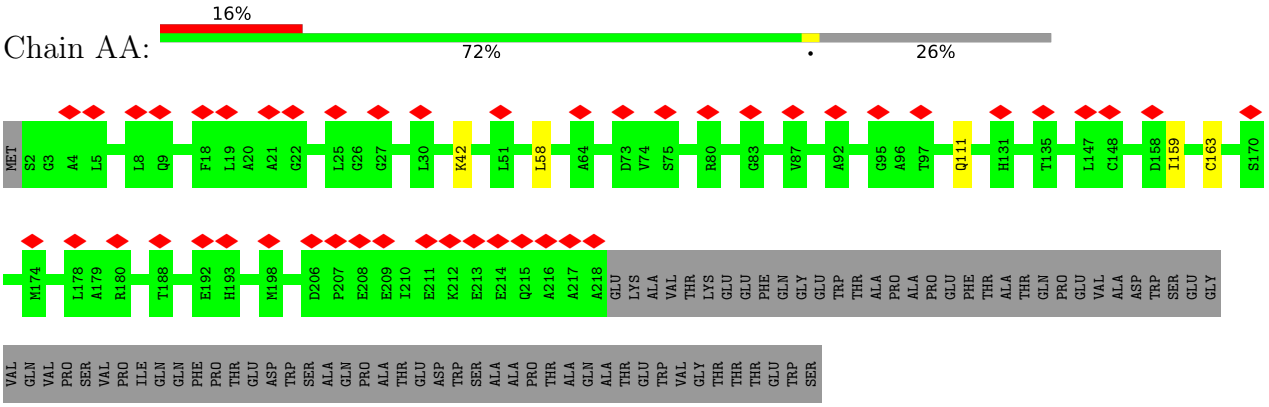

• Molecule 78: 60S ribosomal protein L27a

Chain a:



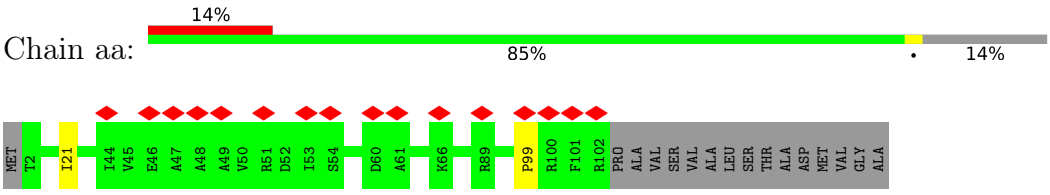

• Molecule 79: 40S_SA_C domain-containing protein

Chain AA:



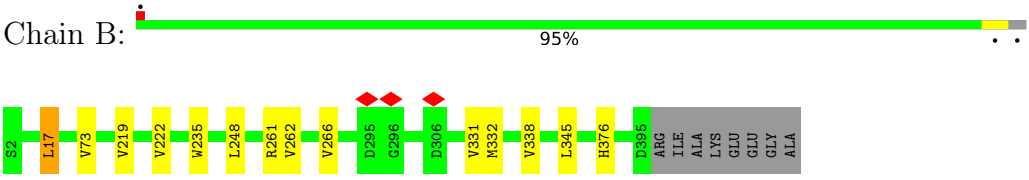

• Molecule 80: 40S ribosomal protein S26

Chain aa:



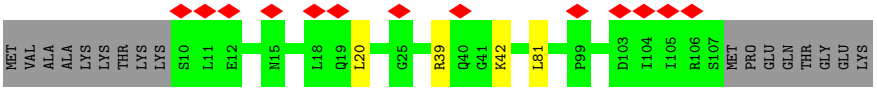

• Molecule 81: uL3

Chain B:

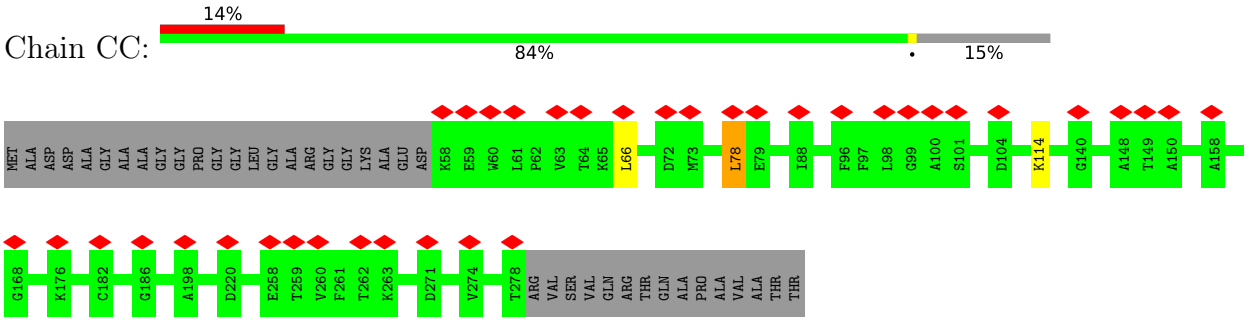



• Molecule 82: eL30

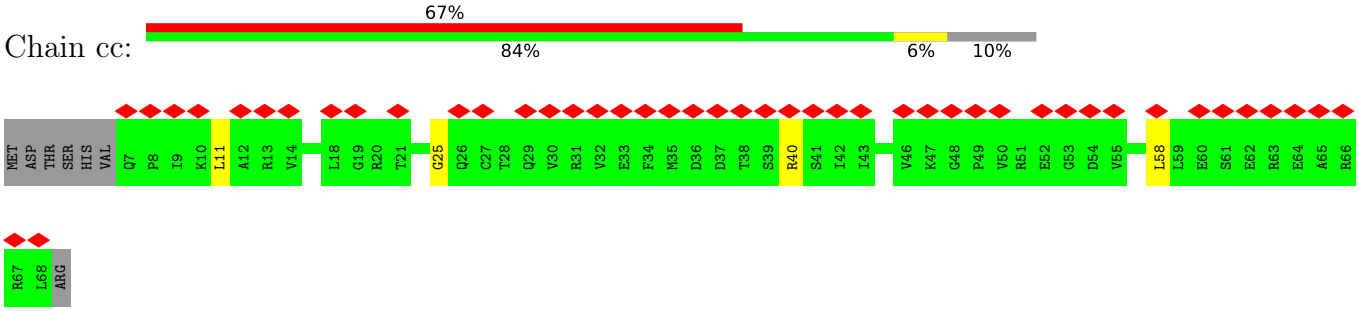
Chain c:




• Molecule 83: 40S ribosomal protein S2




• Molecule 84: 40S ribosomal protein S28



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 18937 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 41.92 | Depositor |
| Minimum defocus (nm) | 400 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 79000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.083 | Depositor |
| Minimum map value | -0.050 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.005 | Depositor |
| Recommended contour level | 0.014 | Depositor |
| Map size (Å) | 405.0, 405.0, 405.0 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.35, 1.35, 1.35 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, MG, ZN, BLS

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 | A | 1.11 | 10/1936 (0.5%) | 0.97 | 2/2596 (0.1%) |
| 2 | C | 1.10 | 13/2937 (0.4%) | 0.98 | 4/3946 (0.1%) |
| 3 | d | 1.02 | 4/903 (0.4%) | 0.95 | 0/1216 |
| 4 | DD | 0.59 | 0/1796 | 1.01 | 5/2417 (0.2%) |
| 5 | dd | 0.64 | 0/470 | 0.96 | 0/623 |
| 6 | D | 0.83 | 0/2437 | 0.87 | 2/3264 (0.1%) |
| 7 | e | 1.18 | 5/1071 (0.5%) | 0.97 | 0/1429 |
| 8 | EE | 0.59 | 0/2118 | 0.90 | 3/2849 (0.1%) |
| 9 | ee | 0.67 | 0/447 | 0.91 | 0/587 |
| 10 | b | 0.82 | 0/861 | 0.91 | 0/1138 |
| 11 | E | 0.88 | 3/1762 (0.2%) | 0.93 | 2/2362 (0.1%) |
| 12 | f | 1.14 | 3/895 (0.3%) | 0.96 | 1/1198 (0.1%) |
| 13 | FF | 0.55 | 0/1492 | 0.92 | 1/2005 (0.0%) |
| 14 | ff | 0.57 | 0/567 | 1.04 | 1/753 (0.1%) |
| 15 | F | 1.17 | 7/1911 (0.4%) | 0.96 | 1/2549 (0.0%) |
| 16 | g | 0.93 | 1/916 (0.1%) | 0.96 | 1/1220 (0.1%) |
| 17 | BB | 0.58 | 0/1756 | 0.90 | 5/2350 (0.2%) |
| 18 | GG | 0.54 | 0/1946 | 0.89 | 1/2590 (0.0%) |
| 19 | gg | 0.46 | 0/2493 | 0.83 | 1/3394 (0.0%) |
| 20 | G | 0.88 | 1/1910 (0.1%) | 0.92 | 1/2569 (0.0%) |
| 21 | h | 0.91 | 1/1021 (0.1%) | 0.97 | 2/1348 (0.1%) |
| 22 | HH | 0.61 | 1/1510 (0.1%) | 0.88 | 4/2022 (0.2%) |
| 23 | hh | 0.67 | 0/353 | 1.37 | 3/547 (0.5%) |
| 24 | bb | 0.56 | 0/665 | 0.84 | 2/891 (0.2%) |
| 25 | H | 0.94 | 1/1535 (0.1%) | 0.88 | 1/2063 (0.0%) |
| 26 | i | 0.90 | 2/841 (0.2%) | 0.94 | 0/1112 |
| 27 | II | 0.62 | 0/1715 | 0.88 | 1/2287 (0.0%) |
| 28 | ii | 0.56 | 0/3361 | 0.98 | 10/4519 (0.2%) |
| 29 | I | 1.01 | 3/1702 (0.2%) | 0.89 | 0/2272 |
| 30 | j | 1.05 | 1/720 (0.1%) | 1.00 | 0/952 |
| 31 | JJ | 0.68 | 0/1550 | 0.86 | 0/2069 |
| 32 | jj | 0.57 | 0/3435 | 0.95 | 8/4633 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | J | 0.77 | 0/1385 | 0.92 | 1/1852 (0.1%) |
| 34 | k | 0.85 | 0/575 | 0.88 | 1/761 (0.1%) |
| 35 | KK | 0.55 | 0/834 | 0.90 | 1/1125 (0.1%) |
| 36 | L | 0.91 | 3/1733 (0.2%) | 0.96 | 0/2316 |
| 37 | l | 0.93 | 0/459 | 0.92 | 1/608 (0.2%) |
| 38 | LL | 0.68 | 0/1195 | 0.85 | 0/1597 |
| 39 | M | 0.94 | 0/1158 | 0.92 | 0/1547 |
| 40 | m | 0.85 | 0/435 | 0.85 | 0/575 |
| 41 | MM | 0.43 | 0/918 | 0.75 | 1/1233 (0.1%) |
| 42 | N | 1.14 | 6/1746 (0.3%) | 0.97 | 2/2338 (0.1%) |
| 43 | n | 0.71 | 0/240 | 1.29 | 2/305 (0.7%) |
| 44 | NN | 0.63 | 0/1226 | 0.88 | 1/1649 (0.1%) |
| 45 | O | 1.16 | 12/1662 (0.7%) | 1.01 | 1/2222 (0.0%) |
| 46 | o | 0.85 | 0/864 | 0.93 | 0/1140 |
| 47 | OO | 0.61 | 0/1029 | 0.94 | 1/1380 (0.1%) |
| 48 | P | 1.07 | 3/1268 (0.2%) | 0.91 | 0/1700 |
| 49 | p | 1.03 | 2/718 (0.3%) | 0.89 | 0/953 |
| 50 | PP | 0.62 | 0/1017 | 1.03 | 2/1358 (0.1%) |
| 51 | Q | 1.13 | 5/1539 (0.3%) | 1.00 | 0/2054 |
| 52 | r | 0.99 | 0/1010 | 0.94 | 1/1354 (0.1%) |
| 53 | QQ | 0.56 | 0/1146 | 0.92 | 1/1534 (0.1%) |
| 54 | R | 0.87 | 3/1524 (0.2%) | 1.01 | 1/2013 (0.0%) |
| 55 | s | 0.55 | 0/1530 | 0.92 | 3/2064 (0.1%) |
| 56 | RR | 0.58 | 0/1082 | 0.87 | 1/1452 (0.1%) |
| 57 | S | 1.08 | 7/1501 (0.5%) | 0.93 | 2/2012 (0.1%) |
| 58 | t | 0.52 | 1/1174 (0.1%) | 0.90 | 2/1582 (0.1%) |
| 59 | SS | 0.56 | 0/1208 | 1.03 | 2/1618 (0.1%) |
| 60 | T | 1.03 | 3/1326 (0.2%) | 0.97 | 1/1770 (0.1%) |
| 61 | TT | 0.55 | 0/1115 | 0.87 | 1/1493 (0.1%) |
| 62 | U | 0.80 | 1/823 (0.1%) | 0.91 | 1/1104 (0.1%) |
| 63 | UU | 0.62 | 0/805 | 0.98 | 2/1081 (0.2%) |
| 64 | V | 1.12 | 1/993 (0.1%) | 0.96 | 0/1332 |
| 65 | VV | 0.60 | 0/643 | 0.81 | 0/860 |
| 66 | W | 0.87 | 1/873 (0.1%) | 0.89 | 0/1158 |
| 67 | 5 | 1.40 | 348/84975 (0.4%) | 1.67 | 1993/132516 (1.5%) |
| 68 | WW | 0.73 | 0/1051 | 0.87 | 0/1406 |
| 69 | X | 0.95 | 1/984 (0.1%) | 0.95 | 1/1323 (0.1%) |
| 70 | 7 | 1.29 | 6/2858 (0.2%) | 1.49 | 26/4455 (0.6%) |
| 71 | XX | 0.73 | 0/1116 | 0.88 | 0/1490 |
| 72 | Y | 1.01 | 1/1132 (0.1%) | 0.98 | 3/1504 (0.2%) |
| 73 | 8 | 1.37 | 9/3581 (0.3%) | 1.65 | 76/5577 (1.4%) |
| 74 | YY | 0.53 | 0/1028 | 0.82 | 0/1366 |
| 75 | Z | 0.92 | 1/1130 (0.1%) | 0.93 | 1/1507 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 76 | 9 | 0.91 | 11/40524 (0.0%) | 1.44 | 428/63134 (0.7%) |
| 77 | ZZ | 0.50 | 0/604 | 0.93 | 0/810 |
| 78 | a | 1.18 | 6/1191 (0.5%) | 0.94 | 0/1590 |
| 79 | AA | 0.61 | 0/1747 | 0.80 | 0/2374 |
| 80 | aa | 0.69 | 0/828 | 0.86 | 0/1109 |
| 81 | B | 1.05 | 11/3240 (0.3%) | 0.95 | 2/4339 (0.0%) |
| 82 | c | 0.85 | 0/771 | 1.09 | 4/1034 (0.4%) |
| 83 | CC | 0.73 | 0/1753 | 0.92 | 2/2369 (0.1%) |
| 84 | cc | 0.61 | 0/490 | 1.07 | 3/656 (0.5%) |
| All | All | 1.10 | 498/234789 (0.2%) | 1.37 | 2633/343469 (0.8%) |

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 |
|---|---|---|---|
| 3 | d | 0 | 1 |
| 53 | QQ | 0 | 1 |
| 67 | 5 | 0 | 7 |
| 71 | XX | 0 | 1 |
| 76 | 9 | 0 | 1 |
| 79 | AA | 0 | 1 |
| All | All | 0 | 12 |

All (498) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2836 | A | N9-C4 | -8.41 | 1.32 | 1.37 |
| 67 | 5 | 1637 | A | N9-C4 | -8.35 | 1.32 | 1.37 |
| 67 | 5 | 1907 | A | N9-C4 | -8.30 | 1.32 | 1.37 |
| 48 | P | 119 | VAL | CB-CG1 | -7.97 | 1.36 | 1.52 |
| 67 | 5 | 2849 | A | N9-C4 | -7.93 | 1.33 | 1.37 |
| 67 | 5 | 1518 | A | N9-C4 | -7.76 | 1.33 | 1.37 |
| 67 | 5 | 39 | A | N7-C5 | -7.61 | 1.34 | 1.39 |
| 81 | B | 262 | VAL | CB-CG2 | -7.56 | 1.36 | 1.52 |
| 67 | 5 | 1352 | C | N1-C6 | -7.55 | 1.32 | 1.37 |
| 67 | 5 | 42 | A | N9-C4 | -7.33 | 1.33 | 1.37 |
| 67 | 5 | 1917 | A | N9-C4 | -7.30 | 1.33 | 1.37 |
| 2 | C | 37 | VAL | CB-CG2 | -7.27 | 1.37 | 1.52 |
| 11 | E | 165 | VAL | CB-CG1 | -7.25 | 1.37 | 1.52 |
| 67 | 5 | 2818 | C | N1-C6 | -7.23 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2844 | A | N9-C4 | -7.21 | 1.33 | 1.37 |
| 67 | 5 | 1655 | C | N1-C6 | -7.14 | 1.32 | 1.37 |
| 12 | f | 29 | LYS | CA-CB | -7.12 | 1.38 | 1.53 |
| 67 | 5 | 4380 | A | C6-N6 | -7.12 | 1.28 | 1.33 |
| 67 | 5 | 3842 | C | N1-C6 | -7.12 | 1.32 | 1.37 |
| 45 | O | 84 | VAL | CB-CG1 | -7.11 | 1.38 | 1.52 |
| 67 | 5 | 1888 | A | N9-C4 | -7.06 | 1.33 | 1.37 |
| 67 | 5 | 3621 | A | N9-C4 | -7.05 | 1.33 | 1.37 |
| 67 | 5 | 2786 | C | N1-C6 | -7.04 | 1.32 | 1.37 |
| 67 | 5 | 1928 | C | N1-C6 | -7.00 | 1.32 | 1.37 |
| 67 | 5 | 65 | A | N9-C4 | -6.97 | 1.33 | 1.37 |
| 81 | B | 332 | MET | CA-CB | -6.95 | 1.38 | 1.53 |
| 67 | 5 | 2072 | C | N1-C6 | -6.94 | 1.32 | 1.37 |
| 67 | 5 | 2785 | C | N1-C6 | -6.92 | 1.32 | 1.37 |
| 67 | 5 | 1505 | C | N1-C6 | -6.89 | 1.33 | 1.37 |
| 67 | 5 | 4214 | A | C6-N6 | -6.81 | 1.28 | 1.33 |
| 67 | 5 | 1661 | C | N1-C6 | -6.81 | 1.33 | 1.37 |
| 67 | 5 | 2579 | G | N9-C4 | -6.80 | 1.32 | 1.38 |
| 67 | 5 | 1331 | C | N1-C6 | -6.75 | 1.33 | 1.37 |
| 67 | 5 | 2317 | C | N1-C6 | -6.73 | 1.33 | 1.37 |
| 15 | F | 107 | VAL | CB-CG2 | -6.72 | 1.38 | 1.52 |
| 67 | 5 | 4206 | C | N1-C6 | -6.72 | 1.33 | 1.37 |
| 67 | 5 | 2423 | A | N9-C4 | -6.71 | 1.33 | 1.37 |
| 67 | 5 | 1503 | A | N9-C4 | -6.70 | 1.33 | 1.37 |
| 67 | 5 | 2335 | C | N1-C6 | -6.70 | 1.33 | 1.37 |
| 67 | 5 | 1520 | C | N1-C6 | -6.69 | 1.33 | 1.37 |
| 11 | E | 178 | VAL | CB-CG2 | -6.69 | 1.38 | 1.52 |
| 67 | 5 | 2410 | C | N1-C6 | -6.66 | 1.33 | 1.37 |
| 67 | 5 | 2334 | C | N1-C6 | -6.66 | 1.33 | 1.37 |
| 67 | 5 | 2025 | A | C6-N6 | -6.65 | 1.28 | 1.33 |
| 67 | 5 | 2446 | C | N1-C6 | -6.65 | 1.33 | 1.37 |
| 67 | 5 | 1633 | G | N9-C8 | -6.60 | 1.33 | 1.37 |
| 73 | 8 | 103 | A | N7-C5 | -6.60 | 1.35 | 1.39 |
| 67 | 5 | 1332 | C | N1-C6 | -6.58 | 1.33 | 1.37 |
| 67 | 5 | 3928 | A | N9-C4 | -6.57 | 1.33 | 1.37 |
| 67 | 5 | 1535 | C | C4-C5 | -6.57 | 1.37 | 1.43 |
| 67 | 5 | 1662 | C | N1-C6 | -6.57 | 1.33 | 1.37 |
| 67 | 5 | 1885 | G | N9-C8 | -6.55 | 1.33 | 1.37 |
| 54 | R | 127 | VAL | CB-CG1 | -6.53 | 1.39 | 1.52 |
| 2 | C | 232 | VAL | CB-CG2 | -6.52 | 1.39 | 1.52 |
| 12 | f | 84 | VAL | CB-CG1 | -6.51 | 1.39 | 1.52 |
| 67 | 5 | 63 | G | N9-C8 | -6.51 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 54 | VAL | CB-CG1 | -6.51 | 1.39 | 1.52 |
| 67 | 5 | 355 | A | C5-C6 | -6.49 | 1.35 | 1.41 |
| 67 | 5 | 1323 | A | N9-C4 | -6.49 | 1.33 | 1.37 |
| 45 | O | 27 | VAL | CB-CG2 | -6.47 | 1.39 | 1.52 |
| 67 | 5 | 1357 | C | N1-C6 | -6.46 | 1.33 | 1.37 |
| 67 | 5 | 1892 | A | C6-N6 | -6.46 | 1.28 | 1.33 |
| 67 | 5 | 1670 | G | N9-C8 | -6.45 | 1.33 | 1.37 |
| 67 | 5 | 4424 | A | N9-C4 | -6.44 | 1.33 | 1.37 |
| 67 | 5 | 338 | A | N9-C4 | -6.44 | 1.33 | 1.37 |
| 2 | C | 246 | VAL | CB-CG1 | -6.41 | 1.39 | 1.52 |
| 70 | 7 | 97 | G | N9-C4 | -6.40 | 1.32 | 1.38 |
| 67 | 5 | 418 | A | C6-N6 | -6.39 | 1.28 | 1.33 |
| 67 | 5 | 1686 | C | N1-C6 | -6.38 | 1.33 | 1.37 |
| 67 | 5 | 4219 | A | N9-C4 | -6.37 | 1.34 | 1.37 |
| 7 | e | 98 | GLU | CB-CG | -6.36 | 1.40 | 1.52 |
| 67 | 5 | 1458 | C | N1-C6 | -6.34 | 1.33 | 1.37 |
| 67 | 5 | 2346 | C | N1-C6 | -6.34 | 1.33 | 1.37 |
| 15 | F | 135 | VAL | CB-CG1 | -6.34 | 1.39 | 1.52 |
| 67 | 5 | 3782 | C | N1-C6 | -6.32 | 1.33 | 1.37 |
| 1 | A | 136 | VAL | CB-CG2 | -6.32 | 1.39 | 1.52 |
| 67 | 5 | 1610 | C | N1-C6 | -6.30 | 1.33 | 1.37 |
| 67 | 5 | 2360 | A | N9-C4 | -6.30 | 1.34 | 1.37 |
| 67 | 5 | 1867 | A | N9-C4 | -6.26 | 1.34 | 1.37 |
| 67 | 5 | 2053 | C | N1-C6 | -6.26 | 1.33 | 1.37 |
| 67 | 5 | 4536 | C | N3-C4 | -6.25 | 1.29 | 1.33 |
| 67 | 5 | 3635 | A | N9-C4 | -6.25 | 1.34 | 1.37 |
| 67 | 5 | 3855 | C | N1-C6 | -6.25 | 1.33 | 1.37 |
| 67 | 5 | 1323 | A | C5-C6 | -6.23 | 1.35 | 1.41 |
| 67 | 5 | 2323 | C | N1-C6 | -6.23 | 1.33 | 1.37 |
| 67 | 5 | 1917 | A | C6-N6 | -6.22 | 1.28 | 1.33 |
| 81 | B | 266 | VAL | CB-CG1 | -6.22 | 1.39 | 1.52 |
| 67 | 5 | 4547 | C | N1-C6 | -6.22 | 1.33 | 1.37 |
| 67 | 5 | 2441 | C | N1-C6 | -6.21 | 1.33 | 1.37 |
| 42 | N | 121 | VAL | CB-CG1 | -6.20 | 1.39 | 1.52 |
| 67 | 5 | 100 | C | N1-C6 | -6.20 | 1.33 | 1.37 |
| 67 | 5 | 350 | C | N1-C6 | -6.20 | 1.33 | 1.37 |
| 67 | 5 | 83 | C | N1-C6 | -6.18 | 1.33 | 1.37 |
| 67 | 5 | 3820 | G | N9-C8 | -6.18 | 1.33 | 1.37 |
| 2 | C | 115 | VAL | CB-CG1 | -6.18 | 1.39 | 1.52 |
| 67 | 5 | 2460 | A | N9-C4 | -6.17 | 1.34 | 1.37 |
| 67 | 5 | 2349 | A | C6-N6 | -6.17 | 1.29 | 1.33 |
| 73 | 8 | 57 | C | N1-C6 | -6.16 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4707 | A | N9-C4 | -6.15 | 1.34 | 1.37 |
| 67 | 5 | 941 | C | N1-C6 | -6.14 | 1.33 | 1.37 |
| 67 | 5 | 1913 | C | N1-C6 | -6.14 | 1.33 | 1.37 |
| 67 | 5 | 5043 | A | N9-C4 | -6.14 | 1.34 | 1.37 |
| 51 | Q | 81 | VAL | CB-CG2 | -6.13 | 1.40 | 1.52 |
| 73 | 8 | 40 | A | N3-C4 | -6.13 | 1.31 | 1.34 |
| 1 | A | 45 | VAL | CB-CG1 | -6.12 | 1.40 | 1.52 |
| 2 | C | 115 | VAL | CB-CG2 | -6.12 | 1.40 | 1.52 |
| 67 | 5 | 1857 | C | N1-C6 | -6.11 | 1.33 | 1.37 |
| 67 | 5 | 4507 | A | N9-C4 | -6.11 | 1.34 | 1.37 |
| 67 | 5 | 1535 | C | N1-C6 | -6.10 | 1.33 | 1.37 |
| 67 | 5 | 4766 | C | N1-C6 | -6.09 | 1.33 | 1.37 |
| 78 | a | 144 | CYS | CA-CB | -6.09 | 1.40 | 1.53 |
| 45 | O | 84 | VAL | CB-CG2 | -6.09 | 1.40 | 1.52 |
| 76 | 9 | 1245 | G | N9-C4 | 6.07 | 1.42 | 1.38 |
| 67 | 5 | 1898 | C | N1-C6 | -6.06 | 1.33 | 1.37 |
| 76 | 9 | 52 | G | N9-C4 | -6.05 | 1.33 | 1.38 |
| 81 | B | 222 | VAL | CB-CG2 | -6.05 | 1.40 | 1.52 |
| 67 | 5 | 4525 | C | N1-C6 | -6.04 | 1.33 | 1.37 |
| 45 | O | 145 | VAL | CB-CG1 | -6.03 | 1.40 | 1.52 |
| 67 | 5 | 1628 | C | C4-C5 | -6.03 | 1.38 | 1.43 |
| 81 | B | 219 | VAL | CB-CG1 | -6.03 | 1.40 | 1.52 |
| 67 | 5 | 67 | C | N1-C6 | -6.02 | 1.33 | 1.37 |
| 67 | 5 | 71 | C | N1-C6 | -6.01 | 1.33 | 1.37 |
| 67 | 5 | 4592 | C | N1-C6 | -6.00 | 1.33 | 1.37 |
| 25 | H | 57 | VAL | CB-CG2 | -5.98 | 1.40 | 1.52 |
| 67 | 5 | 3691 | G | N9-C8 | -5.98 | 1.33 | 1.37 |
| 67 | 5 | 2437 | C | N1-C6 | -5.97 | 1.33 | 1.37 |
| 48 | P | 119 | VAL | CB-CG2 | -5.97 | 1.40 | 1.52 |
| 67 | 5 | 1322 | A | N9-C4 | -5.95 | 1.34 | 1.37 |
| 57 | S | 38 | VAL | CB-CG2 | -5.94 | 1.40 | 1.52 |
| 67 | 5 | 4373 | G | N9-C8 | -5.94 | 1.33 | 1.37 |
| 21 | h | 57 | VAL | CB-CG1 | -5.93 | 1.40 | 1.52 |
| 42 | N | 89 | VAL | CB-CG1 | -5.93 | 1.40 | 1.52 |
| 67 | 5 | 3854 | C | N1-C6 | -5.93 | 1.33 | 1.37 |
| 67 | 5 | 4559 | A | N9-C4 | -5.93 | 1.34 | 1.37 |
| 49 | p | 11 | VAL | CB-CG1 | -5.93 | 1.40 | 1.52 |
| 67 | 5 | 1641 | G | N9-C4 | -5.92 | 1.33 | 1.38 |
| 11 | E | 178 | VAL | CB-CG1 | -5.92 | 1.40 | 1.52 |
| 1 | A | 88 | VAL | CB-CG2 | -5.91 | 1.40 | 1.52 |
| 67 | 5 | 4536 | C | N1-C6 | -5.91 | 1.33 | 1.37 |
| 64 | V | 57 | VAL | CB-CG2 | -5.91 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 73 | 8 | 40 | A | N9-C4 | -5.90 | 1.34 | 1.37 |
| 15 | F | 91 | VAL | CB-CG2 | -5.89 | 1.40 | 1.52 |
| 67 | 5 | 1525 | A | N9-C4 | -5.89 | 1.34 | 1.37 |
| 67 | 5 | 2340 | C | N1-C6 | -5.89 | 1.33 | 1.37 |
| 45 | O | 23 | VAL | CB-CG1 | -5.88 | 1.40 | 1.52 |
| 67 | 5 | 2068 | C | N1-C6 | -5.88 | 1.33 | 1.37 |
| 67 | 5 | 2779 | C | N1-C6 | -5.88 | 1.33 | 1.37 |
| 2 | C | 154 | VAL | CB-CG1 | -5.86 | 1.40 | 1.52 |
| 67 | 5 | 2078 | C | C4-C5 | -5.86 | 1.38 | 1.43 |
| 67 | 5 | 1340 | C | N1-C6 | -5.85 | 1.33 | 1.37 |
| 67 | 5 | 1065 | G | N9-C4 | -5.85 | 1.33 | 1.38 |
| 67 | 5 | 51 | A | C5-C6 | -5.85 | 1.35 | 1.41 |
| 67 | 5 | 299 | C | N1-C6 | -5.84 | 1.33 | 1.37 |
| 70 | 7 | 95 | C | N1-C6 | -5.84 | 1.33 | 1.37 |
| 67 | 5 | 4984 | C | N1-C6 | -5.83 | 1.33 | 1.37 |
| 67 | 5 | 64 | A | C5-C6 | -5.82 | 1.35 | 1.41 |
| 67 | 5 | 2397 | G | N1-C2 | -5.82 | 1.33 | 1.37 |
| 67 | 5 | 2780 | C | N1-C6 | -5.82 | 1.33 | 1.37 |
| 67 | 5 | 1590 | C | N1-C6 | -5.81 | 1.33 | 1.37 |
| 67 | 5 | 41 | C | N1-C6 | -5.81 | 1.33 | 1.37 |
| 67 | 5 | 2068 | C | C4-C5 | -5.80 | 1.38 | 1.43 |
| 67 | 5 | 4688 | C | C4-C5 | -5.79 | 1.38 | 1.43 |
| 73 | 8 | 41 | A | N9-C4 | -5.79 | 1.34 | 1.37 |
| 67 | 5 | 4444 | C | N1-C6 | -5.78 | 1.33 | 1.37 |
| 1 | A | 202 | VAL | CB-CG2 | -5.78 | 1.40 | 1.52 |
| 67 | 5 | 1665 | C | N1-C6 | -5.77 | 1.33 | 1.37 |
| 45 | O | 35 | VAL | CB-CG2 | -5.77 | 1.40 | 1.52 |
| 57 | S | 31 | ARG | CA-CB | -5.76 | 1.41 | 1.53 |
| 67 | 5 | 3858 | C | N1-C6 | -5.75 | 1.33 | 1.37 |
| 67 | 5 | 3882 | C | N1-C6 | -5.75 | 1.33 | 1.37 |
| 67 | 5 | 5004 | C | C4-C5 | -5.75 | 1.38 | 1.43 |
| 67 | 5 | 2815 | A | C5-C6 | -5.74 | 1.35 | 1.41 |
| 67 | 5 | 2604 | C | N1-C6 | -5.74 | 1.33 | 1.37 |
| 51 | Q | 86 | VAL | CB-CG1 | -5.74 | 1.40 | 1.52 |
| 57 | S | 12 | VAL | CB-CG2 | -5.74 | 1.40 | 1.52 |
| 67 | 5 | 4938 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 67 | 5 | 2785 | C | N3-C4 | -5.73 | 1.29 | 1.33 |
| 58 | t | 19 | GLY | C-O | -5.72 | 1.14 | 1.23 |
| 67 | 5 | 1653 | A | C5-C6 | -5.72 | 1.35 | 1.41 |
| 67 | 5 | 4170 | A | C6-N1 | -5.71 | 1.31 | 1.35 |
| 67 | 5 | 4380 | A | C5-C6 | -5.71 | 1.35 | 1.41 |
| 67 | 5 | 3650 | C | C4-C5 | -5.71 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1679 | A | N3-C4 | -5.70 | 1.31 | 1.34 |
| 67 | 5 | 4767 | C | N1-C6 | -5.70 | 1.33 | 1.37 |
| 67 | 5 | 2532 | C | N1-C6 | -5.70 | 1.33 | 1.37 |
| 67 | 5 | 3727 | A | N9-C4 | -5.70 | 1.34 | 1.37 |
| 67 | 5 | 2464 | C | N1-C6 | -5.70 | 1.33 | 1.37 |
| 76 | 9 | 1853 | C | N1-C6 | -5.70 | 1.33 | 1.37 |
| 29 | I | 38 | ARG | CA-CB | -5.70 | 1.41 | 1.53 |
| 78 | a | 124 | VAL | CB-CG1 | -5.68 | 1.41 | 1.52 |
| 67 | 5 | 293 | G | N9-C8 | -5.68 | 1.33 | 1.37 |
| 67 | 5 | 3852 | A | N9-C4 | -5.68 | 1.34 | 1.37 |
| 67 | 5 | 4662 | C | N1-C6 | -5.67 | 1.33 | 1.37 |
| 2 | C | 40 | VAL | CB-CG1 | -5.66 | 1.41 | 1.52 |
| 67 | 5 | 1350 | C | N1-C6 | -5.66 | 1.33 | 1.37 |
| 67 | 5 | 1938 | C | N1-C6 | -5.66 | 1.33 | 1.37 |
| 67 | 5 | 2739 | C | N1-C6 | -5.66 | 1.33 | 1.37 |
| 67 | 5 | 4305 | G | N7-C5 | -5.66 | 1.35 | 1.39 |
| 81 | B | 266 | VAL | CB-CG2 | -5.65 | 1.41 | 1.52 |
| 67 | 5 | 4487 | A | N9-C4 | -5.65 | 1.34 | 1.37 |
| 51 | Q | 47 | VAL | CB-CG2 | -5.64 | 1.41 | 1.52 |
| 67 | 5 | 4223 | C | N1-C6 | -5.64 | 1.33 | 1.37 |
| 67 | 5 | 418 | A | C6-N1 | -5.63 | 1.31 | 1.35 |
| 76 | 9 | 813 | A | N9-C4 | -5.63 | 1.34 | 1.37 |
| 67 | 5 | 410 | A | N9-C4 | -5.63 | 1.34 | 1.37 |
| 1 | A | 88 | VAL | CB-CG1 | -5.62 | 1.41 | 1.52 |
| 67 | 5 | 4716 | C | N1-C6 | -5.62 | 1.33 | 1.37 |
| 73 | 8 | 26 | C | C4-C5 | -5.62 | 1.38 | 1.43 |
| 67 | 5 | 3864 | C | N1-C6 | -5.62 | 1.33 | 1.37 |
| 67 | 5 | 94 | A | N9-C4 | -5.61 | 1.34 | 1.37 |
| 67 | 5 | 1900 | C | N1-C6 | -5.61 | 1.33 | 1.37 |
| 75 | Z | 74 | VAL | CB-CG1 | -5.61 | 1.41 | 1.52 |
| 67 | 5 | 3643 | A | N9-C4 | -5.60 | 1.34 | 1.37 |
| 67 | 5 | 1499 | C | N1-C6 | -5.60 | 1.33 | 1.37 |
| 67 | 5 | 2858 | A | N9-C4 | -5.60 | 1.34 | 1.37 |
| 67 | 5 | 1515 | A | C6-N6 | -5.60 | 1.29 | 1.33 |
| 42 | N | 192 | TRP | CB-CG | -5.59 | 1.40 | 1.50 |
| 36 | L | 70 | VAL | CB-CG1 | -5.58 | 1.41 | 1.52 |
| 67 | 5 | 2351 | C | N1-C6 | -5.58 | 1.33 | 1.37 |
| 7 | e | 45 | VAL | CB-CG2 | -5.58 | 1.41 | 1.52 |
| 15 | F | 122 | VAL | CB-CG2 | -5.57 | 1.41 | 1.52 |
| 67 | 5 | 4393 | G | N9-C8 | -5.57 | 1.33 | 1.37 |
| 45 | O | 104 | VAL | CB-CG2 | -5.57 | 1.41 | 1.52 |
| 76 | 9 | 1383 | A | N9-C4 | -5.57 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4319 | C | N1-C6 | -5.57 | 1.33 | 1.37 |
| 48 | P | 24 | VAL | CB-CG2 | -5.56 | 1.41 | 1.52 |
| 67 | 5 | 4519 | C | N1-C6 | -5.56 | 1.33 | 1.37 |
| 67 | 5 | 27 | C | N1-C6 | -5.55 | 1.33 | 1.37 |
| 67 | 5 | 2392 | C | C4-C5 | -5.55 | 1.38 | 1.43 |
| 67 | 5 | 3896 | C | N1-C6 | -5.55 | 1.33 | 1.37 |
| 67 | 5 | 4562 | C | N1-C6 | -5.54 | 1.33 | 1.37 |
| 67 | 5 | 2783 | A | N9-C4 | -5.54 | 1.34 | 1.37 |
| 67 | 5 | 3911 | C | C4-C5 | -5.54 | 1.38 | 1.43 |
| 67 | 5 | 4710 | C | N1-C6 | -5.52 | 1.33 | 1.37 |
| 2 | C | 183 | VAL | CB-CG1 | -5.52 | 1.41 | 1.52 |
| 67 | 5 | 2836 | A | C5-C6 | -5.51 | 1.36 | 1.41 |
| 67 | 5 | 1626 | G | N9-C4 | -5.51 | 1.33 | 1.38 |
| 67 | 5 | 3633 | C | N1-C6 | -5.51 | 1.33 | 1.37 |
| 67 | 5 | 3893 | C | N1-C6 | -5.51 | 1.33 | 1.37 |
| 2 | C | 79 | VAL | CB-CG1 | -5.50 | 1.41 | 1.52 |
| 67 | 5 | 1666 | C | N1-C6 | -5.50 | 1.33 | 1.37 |
| 67 | 5 | 4428 | A | N9-C4 | -5.50 | 1.34 | 1.37 |
| 3 | d | 72 | VAL | CB-CG1 | -5.50 | 1.41 | 1.52 |
| 67 | 5 | 53 | C | N1-C6 | -5.49 | 1.33 | 1.37 |
| 72 | Y | 58 | VAL | CB-CG1 | -5.49 | 1.41 | 1.52 |
| 67 | 5 | 41 | C | C4-C5 | -5.49 | 1.38 | 1.43 |
| 67 | 5 | 2783 | A | C6-N6 | -5.49 | 1.29 | 1.33 |
| 67 | 5 | 38 | A | C5-C6 | -5.48 | 1.36 | 1.41 |
| 67 | 5 | 2051 | C | C4-C5 | -5.48 | 1.38 | 1.43 |
| 67 | 5 | 5016 | A | C5-C6 | -5.48 | 1.36 | 1.41 |
| 67 | 5 | 1898 | C | C4-C5 | -5.48 | 1.38 | 1.43 |
| 81 | B | 262 | VAL | CB-CG1 | -5.47 | 1.41 | 1.52 |
| 67 | 5 | 56 | A | N9-C4 | -5.47 | 1.34 | 1.37 |
| 67 | 5 | 3910 | C | C4-C5 | -5.47 | 1.38 | 1.43 |
| 67 | 5 | 4561 | C | N1-C6 | -5.47 | 1.33 | 1.37 |
| 81 | B | 73 | VAL | CB-CG2 | -5.47 | 1.41 | 1.52 |
| 81 | B | 331 | VAL | CB-CG2 | -5.46 | 1.41 | 1.52 |
| 67 | 5 | 1662 | C | C4-C5 | -5.46 | 1.38 | 1.43 |
| 67 | 5 | 1327 | C | C4-C5 | -5.46 | 1.38 | 1.43 |
| 67 | 5 | 3702 | A | N9-C4 | -5.46 | 1.34 | 1.37 |
| 67 | 5 | 2772 | C | N1-C6 | -5.45 | 1.33 | 1.37 |
| 67 | 5 | 1580 | C | C4-C5 | -5.45 | 1.38 | 1.43 |
| 67 | 5 | 1893 | C | N1-C6 | -5.45 | 1.33 | 1.37 |
| 67 | 5 | 1872 | G | N9-C4 | -5.44 | 1.33 | 1.38 |
| 67 | 5 | 3687 | A | N9-C4 | -5.44 | 1.34 | 1.37 |
| 3 | d | 106 | VAL | CB-CG1 | -5.44 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1847 | C | N1-C6 | -5.44 | 1.33 | 1.37 |
| 67 | 5 | 1306 | C | C4-C5 | -5.43 | 1.38 | 1.43 |
| 1 | A | 202 | VAL | CB-CG1 | -5.43 | 1.41 | 1.52 |
| 67 | 5 | 4502 | C | N1-C6 | -5.43 | 1.33 | 1.37 |
| 29 | I | 96 | VAL | CB-CG2 | -5.42 | 1.41 | 1.52 |
| 67 | 5 | 2745 | A | N9-C4 | -5.42 | 1.34 | 1.37 |
| 67 | 5 | 3909 | C | C4-N4 | -5.42 | 1.29 | 1.33 |
| 67 | 5 | 1427 | A | N9-C4 | -5.42 | 1.34 | 1.37 |
| 7 | e | 79 | VAL | CB-CG1 | -5.42 | 1.41 | 1.52 |
| 67 | 5 | 2641 | A | N9-C4 | -5.42 | 1.34 | 1.37 |
| 73 | 8 | 18 | U | N1-C2 | -5.42 | 1.33 | 1.38 |
| 76 | 9 | 1563 | G | N9-C4 | -5.42 | 1.33 | 1.38 |
| 78 | a | 124 | VAL | CB-CG2 | -5.42 | 1.41 | 1.52 |
| 67 | 5 | 1397 | A | C6-N6 | -5.41 | 1.29 | 1.33 |
| 67 | 5 | 1888 | A | N3-C4 | -5.41 | 1.31 | 1.34 |
| 67 | 5 | 2290 | C | N1-C6 | -5.41 | 1.33 | 1.37 |
| 67 | 5 | 4724 | A | C6-N6 | -5.41 | 1.29 | 1.33 |
| 67 | 5 | 1648 | C | N1-C6 | -5.41 | 1.33 | 1.37 |
| 67 | 5 | 1654 | G | N9-C8 | -5.41 | 1.34 | 1.37 |
| 67 | 5 | 1631 | A | N9-C8 | -5.41 | 1.33 | 1.37 |
| 57 | S | 67 | VAL | CB-CG1 | -5.40 | 1.41 | 1.52 |
| 67 | 5 | 2849 | A | C5-C4 | -5.40 | 1.34 | 1.38 |
| 67 | 5 | 3879 | G | N9-C4 | -5.39 | 1.33 | 1.38 |
| 7 | e | 45 | VAL | CB-CG1 | -5.39 | 1.41 | 1.52 |
| 81 | B | 235 | TRP | CB-CG | -5.39 | 1.40 | 1.50 |
| 67 | 5 | 1469 | C | N1-C6 | -5.39 | 1.33 | 1.37 |
| 67 | 5 | 1535 | C | C4-N4 | -5.39 | 1.29 | 1.33 |
| 67 | 5 | 2743 | A | C6-N6 | -5.38 | 1.29 | 1.33 |
| 2 | C | 183 | VAL | CB-CG2 | -5.38 | 1.41 | 1.52 |
| 67 | 5 | 1628 | C | N1-C6 | -5.38 | 1.33 | 1.37 |
| 45 | O | 23 | VAL | CB-CG2 | -5.38 | 1.41 | 1.52 |
| 57 | S | 39 | VAL | CB-CG2 | -5.38 | 1.41 | 1.52 |
| 67 | 5 | 2791 | C | N1-C6 | -5.38 | 1.33 | 1.37 |
| 67 | 5 | 4590 | A | N9-C4 | -5.37 | 1.34 | 1.37 |
| 67 | 5 | 360 | A | C6-N6 | -5.36 | 1.29 | 1.33 |
| 67 | 5 | 1577 | G | N9-C8 | -5.36 | 1.34 | 1.37 |
| 67 | 5 | 4170 | A | C6-N6 | -5.36 | 1.29 | 1.33 |
| 67 | 5 | 210 | C | N1-C6 | -5.35 | 1.33 | 1.37 |
| 67 | 5 | 289 | C | N1-C6 | -5.35 | 1.33 | 1.37 |
| 67 | 5 | 1879 | C | C4-C5 | -5.35 | 1.38 | 1.43 |
| 1 | A | 235 | VAL | CB-CG2 | -5.35 | 1.41 | 1.52 |
| 67 | 5 | 33 | A | N9-C4 | -5.35 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 410 | A | C6-N6 | -5.34 | 1.29 | 1.33 |
| 67 | 5 | 4564 | A | N9-C4 | -5.34 | 1.34 | 1.37 |
| 67 | 5 | 2071 | A | N9-C8 | -5.33 | 1.33 | 1.37 |
| 67 | 5 | 1632 | A | N7-C5 | -5.33 | 1.36 | 1.39 |
| 67 | 5 | 238 | C | N1-C6 | -5.33 | 1.33 | 1.37 |
| 73 | 8 | 105 | C | N1-C6 | -5.32 | 1.33 | 1.37 |
| 51 | Q | 148 | VAL | CB-CG2 | -5.32 | 1.41 | 1.52 |
| 57 | S | 62 | VAL | CB-CG2 | -5.32 | 1.41 | 1.52 |
| 67 | 5 | 355 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 67 | 5 | 4565 | C | C4-C5 | -5.32 | 1.38 | 1.43 |
| 78 | a | 111 | VAL | CB-CG1 | -5.32 | 1.41 | 1.52 |
| 67 | 5 | 2509 | C | C4-C5 | -5.32 | 1.38 | 1.43 |
| 67 | 5 | 4087 | G | N9-C4 | -5.31 | 1.33 | 1.38 |
| 67 | 5 | 2797 | C | N1-C6 | -5.30 | 1.33 | 1.37 |
| 76 | 9 | 1469 | A | N9-C4 | 5.30 | 1.41 | 1.37 |
| 67 | 5 | 1541 | C | N1-C6 | -5.30 | 1.33 | 1.37 |
| 16 | g | 87 | VAL | CB-CG2 | -5.30 | 1.41 | 1.52 |
| 30 | j | 70 | VAL | CB-CG2 | -5.30 | 1.41 | 1.52 |
| 67 | 5 | 3876 | A | C6-N1 | -5.29 | 1.31 | 1.35 |
| 45 | O | 34 | VAL | CB-CG1 | -5.29 | 1.41 | 1.52 |
| 67 | 5 | 1346 | C | N1-C6 | -5.29 | 1.33 | 1.37 |
| 67 | 5 | 3774 | A | C5-C6 | -5.29 | 1.36 | 1.41 |
| 70 | 7 | 10 | C | N1-C6 | -5.29 | 1.33 | 1.37 |
| 15 | F | 116 | ILE | CB-CG2 | -5.28 | 1.36 | 1.52 |
| 67 | 5 | 4184 | G | N9-C4 | -5.28 | 1.33 | 1.38 |
| 49 | p | 64 | VAL | CB-CG2 | -5.28 | 1.41 | 1.52 |
| 54 | R | 22 | VAL | CB-CG1 | -5.28 | 1.41 | 1.52 |
| 67 | 5 | 1920 | C | N1-C6 | -5.28 | 1.33 | 1.37 |
| 67 | 5 | 2392 | C | N1-C6 | -5.28 | 1.33 | 1.37 |
| 67 | 5 | 1908 | A | C5-C6 | -5.27 | 1.36 | 1.41 |
| 67 | 5 | 2770 | C | N1-C6 | -5.27 | 1.33 | 1.37 |
| 29 | I | 126 | VAL | CB-CG1 | -5.27 | 1.41 | 1.52 |
| 26 | i | 76 | ARG | CB-CG | -5.27 | 1.38 | 1.52 |
| 67 | 5 | 3672 | G | N9-C4 | -5.27 | 1.33 | 1.38 |
| 67 | 5 | 1599 | G | N1-C2 | -5.27 | 1.33 | 1.37 |
| 67 | 5 | 2422 | C | N1-C6 | -5.27 | 1.33 | 1.37 |
| 15 | F | 104 | VAL | CB-CG1 | -5.26 | 1.41 | 1.52 |
| 70 | 7 | 97 | G | C2-N3 | -5.26 | 1.28 | 1.32 |
| 60 | T | 76 | VAL | CB-CG2 | -5.26 | 1.41 | 1.52 |
| 67 | 5 | 92 | C | N1-C6 | -5.26 | 1.33 | 1.37 |
| 67 | 5 | 2268 | A | N9-C4 | -5.26 | 1.34 | 1.37 |
| 67 | 5 | 2851 | G | N9-C8 | -5.26 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4186 | A | N3-C4 | -5.26 | 1.31 | 1.34 |
| 67 | 5 | 3655 | C | N1-C6 | -5.25 | 1.33 | 1.37 |
| 45 | O | 35 | VAL | CB-CG1 | -5.25 | 1.41 | 1.52 |
| 81 | B | 338 | VAL | CB-CG1 | -5.25 | 1.41 | 1.52 |
| 67 | 5 | 2075 | G | N9-C8 | -5.25 | 1.34 | 1.37 |
| 66 | W | 53 | VAL | CB-CG2 | -5.24 | 1.41 | 1.52 |
| 67 | 5 | 4533 | A | C5-C6 | -5.24 | 1.36 | 1.41 |
| 67 | 5 | 1387 | A | C5-C6 | -5.24 | 1.36 | 1.41 |
| 67 | 5 | 1521 | C | C4-C5 | -5.24 | 1.38 | 1.43 |
| 67 | 5 | 1879 | C | N1-C6 | -5.24 | 1.34 | 1.37 |
| 60 | T | 76 | VAL | CB-CG1 | -5.23 | 1.41 | 1.52 |
| 67 | 5 | 422 | C | C4-C5 | -5.23 | 1.38 | 1.43 |
| 67 | 5 | 2529 | A | N9-C4 | -5.23 | 1.34 | 1.37 |
| 67 | 5 | 4080 | C | N1-C6 | -5.23 | 1.34 | 1.37 |
| 15 | F | 135 | VAL | CB-CG2 | -5.23 | 1.41 | 1.52 |
| 67 | 5 | 222 | C | N1-C6 | -5.23 | 1.34 | 1.37 |
| 42 | N | 25 | VAL | CB-CG2 | -5.23 | 1.41 | 1.52 |
| 67 | 5 | 1795 | A | C6-N6 | -5.23 | 1.29 | 1.33 |
| 67 | 5 | 1339 | U | C2-N3 | -5.22 | 1.34 | 1.37 |
| 67 | 5 | 1668 | A | C6-N1 | -5.22 | 1.31 | 1.35 |
| 45 | O | 33 | VAL | CB-CG2 | -5.22 | 1.41 | 1.52 |
| 78 | a | 103 | VAL | CB-CG2 | -5.21 | 1.42 | 1.52 |
| 67 | 5 | 1942 | A | N9-C4 | -5.21 | 1.34 | 1.37 |
| 67 | 5 | 1884 | C | N1-C6 | -5.21 | 1.34 | 1.37 |
| 67 | 5 | 3859 | G | N9-C8 | -5.21 | 1.34 | 1.37 |
| 67 | 5 | 2881 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 67 | 5 | 2069 | A | N9-C4 | -5.20 | 1.34 | 1.37 |
| 1 | A | 207 | VAL | CB-CG2 | -5.20 | 1.42 | 1.52 |
| 36 | L | 25 | TRP | CB-CG | -5.20 | 1.40 | 1.50 |
| 22 | HH | 100 | ILE | C-N | 5.20 | 1.46 | 1.34 |
| 67 | 5 | 4653 | C | N1-C6 | -5.19 | 1.34 | 1.37 |
| 67 | 5 | 4671 | C | N1-C6 | -5.19 | 1.34 | 1.37 |
| 67 | 5 | 4883 | C | N1-C6 | -5.19 | 1.34 | 1.37 |
| 67 | 5 | 362 | A | N9-C4 | -5.18 | 1.34 | 1.37 |
| 67 | 5 | 1313 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 67 | 5 | 4485 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 67 | 5 | 1524 | A | N9-C4 | -5.18 | 1.34 | 1.37 |
| 67 | 5 | 3869 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 67 | 5 | 3700 | C | N1-C6 | -5.17 | 1.34 | 1.37 |
| 3 | d | 86 | VAL | CB-CG1 | -5.17 | 1.42 | 1.52 |
| 67 | 5 | 26 | C | N1-C6 | -5.17 | 1.34 | 1.37 |
| 67 | 5 | 414 | C | N1-C6 | -5.17 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2393 | C | N1-C6 | -5.17 | 1.34 | 1.37 |
| 67 | 5 | 4982 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 67 | 5 | 4715 | C | C4-C5 | -5.17 | 1.38 | 1.43 |
| 67 | 5 | 81 | C | C4-C5 | -5.16 | 1.38 | 1.43 |
| 67 | 5 | 1331 | C | C4-C5 | -5.16 | 1.38 | 1.43 |
| 67 | 5 | 87 | A | N9-C8 | -5.15 | 1.33 | 1.37 |
| 76 | 9 | 628 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 67 | 5 | 323 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 67 | 5 | 33 | A | C6-N6 | -5.14 | 1.29 | 1.33 |
| 67 | 5 | 357 | U | N1-C6 | -5.14 | 1.33 | 1.38 |
| 7 | e | 79 | VAL | CB-CG2 | -5.14 | 1.42 | 1.52 |
| 67 | 5 | 1895 | G | N9-C8 | -5.14 | 1.34 | 1.37 |
| 67 | 5 | 2338 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 42 | N | 59 | TYR | CD1-CE1 | -5.14 | 1.31 | 1.39 |
| 67 | 5 | 4325 | A | C6-N6 | -5.14 | 1.29 | 1.33 |
| 54 | R | 22 | VAL | CB-CG2 | -5.13 | 1.42 | 1.52 |
| 67 | 5 | 1631 | A | N9-C4 | -5.13 | 1.34 | 1.37 |
| 67 | 5 | 4979 | A | C5-C6 | -5.13 | 1.36 | 1.41 |
| 70 | 7 | 111 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 67 | 5 | 1659 | U | N1-C2 | -5.13 | 1.33 | 1.38 |
| 67 | 5 | 1785 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 67 | 5 | 2397 | G | C6-N1 | -5.13 | 1.35 | 1.39 |
| 67 | 5 | 4318 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 12 | f | 84 | VAL | CB-CG2 | -5.12 | 1.42 | 1.52 |
| 67 | 5 | 4720 | C | N1-C6 | -5.12 | 1.34 | 1.37 |
| 67 | 5 | 332 | C | C4-C5 | -5.12 | 1.38 | 1.43 |
| 67 | 5 | 4313 | A | N9-C4 | -5.12 | 1.34 | 1.37 |
| 67 | 5 | 4533 | A | N7-C5 | -5.12 | 1.36 | 1.39 |
| 67 | 5 | 21 | G | N9-C8 | -5.11 | 1.34 | 1.37 |
| 67 | 5 | 1674 | C | C4-C5 | -5.11 | 1.38 | 1.43 |
| 67 | 5 | 1669 | A | C6-N6 | -5.11 | 1.29 | 1.33 |
| 67 | 5 | 2039 | G | N1-C2 | -5.11 | 1.33 | 1.37 |
| 67 | 5 | 2853 | C | N1-C6 | -5.11 | 1.34 | 1.37 |
| 67 | 5 | 2279 | A | N9-C4 | -5.11 | 1.34 | 1.37 |
| 67 | 5 | 1857 | C | C4-C5 | -5.10 | 1.38 | 1.43 |
| 67 | 5 | 4761 | G | N9-C4 | -5.10 | 1.33 | 1.38 |
| 67 | 5 | 4466 | C | N1-C6 | -5.10 | 1.34 | 1.37 |
| 69 | X | 100 | VAL | CB-CG1 | -5.10 | 1.42 | 1.52 |
| 2 | C | 73 | VAL | CB-CG2 | -5.10 | 1.42 | 1.52 |
| 36 | L | 79 | GLU | CB-CG | -5.10 | 1.42 | 1.52 |
| 67 | 5 | 2438 | A | C5-C6 | -5.10 | 1.36 | 1.41 |
| 67 | 5 | 39 | A | C8-N7 | -5.10 | 1.27 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 422 | C | N1-C6 | -5.10 | 1.34 | 1.37 |
| 67 | 5 | 3654 | G | N3-C4 | -5.10 | 1.31 | 1.35 |
| 1 | A | 235 | VAL | CB-CG1 | -5.09 | 1.42 | 1.52 |
| 20 | G | 196 | VAL | CB-CG2 | -5.09 | 1.42 | 1.52 |
| 51 | Q | 82 | VAL | CB-CG2 | -5.09 | 1.42 | 1.52 |
| 67 | 5 | 2458 | C | N1-C6 | -5.08 | 1.34 | 1.37 |
| 67 | 5 | 47 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 67 | 5 | 1681 | G | N9-C8 | -5.08 | 1.34 | 1.37 |
| 67 | 5 | 4561 | C | N3-C4 | -5.08 | 1.30 | 1.33 |
| 67 | 5 | 4195 | G | C6-N1 | -5.08 | 1.35 | 1.39 |
| 57 | S | 38 | VAL | CB-CG1 | -5.08 | 1.42 | 1.52 |
| 45 | O | 33 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 67 | 5 | 4386 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 73 | 8 | 140 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 2 | C | 37 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 67 | 5 | 1354 | A | C6-N6 | -5.07 | 1.29 | 1.33 |
| 67 | 5 | 4862 | G | N9-C4 | -5.07 | 1.33 | 1.38 |
| 67 | 5 | 941 | C | C4-C5 | -5.07 | 1.38 | 1.43 |
| 67 | 5 | 2078 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 67 | 5 | 5050 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 62 | U | 49 | VAL | CB-CG2 | -5.06 | 1.42 | 1.52 |
| 67 | 5 | 2802 | C | N1-C6 | -5.06 | 1.34 | 1.37 |
| 67 | 5 | 1279 | A | N9-C4 | -5.06 | 1.34 | 1.37 |
| 67 | 5 | 1788 | A | N9-C4 | -5.05 | 1.34 | 1.37 |
| 67 | 5 | 4456 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 67 | 5 | 39 | A | C5-C6 | -5.05 | 1.36 | 1.41 |
| 67 | 5 | 4507 | A | N3-C4 | -5.05 | 1.31 | 1.34 |
| 67 | 5 | 4488 | A | N9-C4 | -5.05 | 1.34 | 1.37 |
| 70 | 7 | 14 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 67 | 5 | 358 | C | N1-C6 | -5.04 | 1.34 | 1.37 |
| 76 | 9 | 1200 | A | N9-C4 | -5.04 | 1.34 | 1.37 |
| 67 | 5 | 1276 | C | N1-C6 | -5.04 | 1.34 | 1.37 |
| 67 | 5 | 4582 | C | N1-C6 | -5.04 | 1.34 | 1.37 |
| 60 | T | 75 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |
| 67 | 5 | 1521 | C | N1-C6 | -5.04 | 1.34 | 1.37 |
| 67 | 5 | 2321 | G | N9-C4 | -5.03 | 1.33 | 1.38 |
| 67 | 5 | 2409 | U | N1-C6 | -5.03 | 1.33 | 1.38 |
| 67 | 5 | 3846 | C | N1-C6 | -5.03 | 1.34 | 1.37 |
| 1 | A | 169 | VAL | CB-CG1 | -5.03 | 1.42 | 1.52 |
| 67 | 5 | 2295 | C | N1-C6 | -5.03 | 1.34 | 1.37 |
| 67 | 5 | 4535 | A | N3-C4 | -5.03 | 1.31 | 1.34 |
| 67 | 5 | 4508 | C | C4-C5 | -5.03 | 1.39 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | N | 155 | VAL | CB-CG2 | -5.03 | 1.42 | 1.52 |
| 67 | 5 | 101 | A | C5-C6 | -5.03 | 1.36 | 1.41 |
| 67 | 5 | 1507 | C | C4-C5 | -5.03 | 1.39 | 1.43 |
| 67 | 5 | 1855 | G | N9-C8 | -5.03 | 1.34 | 1.37 |
| 67 | 5 | 2381 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 67 | 5 | 2461 | G | N9-C8 | -5.02 | 1.34 | 1.37 |
| 3 | d | 36 | VAL | CB-CG2 | -5.02 | 1.42 | 1.52 |
| 67 | 5 | 1518 | A | C6-N6 | -5.02 | 1.29 | 1.33 |
| 67 | 5 | 3653 | A | N7-C5 | -5.02 | 1.36 | 1.39 |
| 67 | 5 | 1460 | C | C4-C5 | -5.02 | 1.39 | 1.43 |
| 67 | 5 | 2449 | A | C6-N6 | -5.02 | 1.29 | 1.33 |
| 67 | 5 | 2583 | C | N1-C6 | -5.02 | 1.34 | 1.37 |
| 67 | 5 | 4313 | A | N3-C4 | -5.02 | 1.31 | 1.34 |
| 76 | 9 | 330 | G | N9-C4 | -5.02 | 1.33 | 1.38 |
| 67 | 5 | 1396 | G | N9-C8 | -5.01 | 1.34 | 1.37 |
| 76 | 9 | 1719 | A | N9-C4 | -5.01 | 1.34 | 1.37 |
| 67 | 5 | 3903 | A | C5-C6 | -5.01 | 1.36 | 1.41 |
| 26 | i | 77 | VAL | CB-CG2 | -5.01 | 1.42 | 1.52 |
| 67 | 5 | 3747 | A | N9-C4 | -5.00 | 1.34 | 1.37 |
| 67 | 5 | 79 | C | N1-C6 | -5.00 | 1.34 | 1.37 |
| 67 | 5 | 1908 | A | C6-N6 | -5.00 | 1.29 | 1.33 |
| 78 | a | 61 | TYR | CE1-CZ | -5.00 | 1.32 | 1.38 |

All (2633) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 3911 | C | C6-N1-C2 | -12.96 | 115.12 | 120.30 |
| 67 | 5 | 1535 | C | C5-C4-N4 | -12.52 | 111.44 | 120.20 |
| 67 | 5 | 1081 | C | C6-N1-C2 | -12.39 | 115.34 | 120.30 |
| 67 | 5 | 4723 | A | C6-N1-C2 | -12.38 | 111.17 | 118.60 |
| 67 | 5 | 143 | C | O4'-C1'-N1 | 12.29 | 118.03 | 108.20 |
| 73 | 8 | 103 | A | N1-C6-N6 | 12.25 | 125.95 | 118.60 |
| 67 | 5 | 38 | A | N1-C6-N6 | 11.79 | 125.67 | 118.60 |
| 76 | 9 | 1215 | C | C6-N1-C2 | -11.57 | 115.67 | 120.30 |
| 67 | 5 | 3653 | A | C8-N9-C4 | -11.47 | 101.21 | 105.80 |
| 67 | 5 | 3910 | C | C6-N1-C2 | -11.29 | 115.78 | 120.30 |
| 67 | 5 | 41 | C | N1-C2-O2 | 11.10 | 125.56 | 118.90 |
| 67 | 5 | 3653 | A | C8-N9-C1' | -11.09 | 107.75 | 127.70 |
| 67 | 5 | 1308 | C | C6-N1-C2 | -11.07 | 115.87 | 120.30 |
| 67 | 5 | 2579 | G | N3-C4-N9 | -11.02 | 119.39 | 126.00 |
| 67 | 5 | 5004 | C | C5-C4-N4 | -10.98 | 112.52 | 120.20 |
| 70 | 7 | 97 | G | N3-C4-N9 | -10.67 | 119.60 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 3909 | C | N3-C4-C5 | 10.65 | 126.16 | 121.90 |
| 67 | 5 | 2465 | C | N1-C2-O2 | 10.52 | 125.21 | 118.90 |
| 67 | 5 | 1628 | C | C5-C4-N4 | -10.34 | 112.96 | 120.20 |
| 67 | 5 | 1081 | C | C2-N1-C1' | 10.32 | 130.15 | 118.80 |
| 67 | 5 | 30 | C | N1-C2-O2 | 10.31 | 125.09 | 118.90 |
| 67 | 5 | 1653 | A | N1-C6-N6 | 10.18 | 124.71 | 118.60 |
| 67 | 5 | 4536 | C | N3-C2-O2 | -10.12 | 114.82 | 121.90 |
| 67 | 5 | 2799 | G | C4-N9-C1' | 10.11 | 139.64 | 126.50 |
| 67 | 5 | 1812 | C | C2-N1-C1' | 10.07 | 129.88 | 118.80 |
| 67 | 5 | 2785 | C | N1-C2-O2 | 10.00 | 124.90 | 118.90 |
| 67 | 5 | 355 | A | N1-C6-N6 | 10.00 | 124.60 | 118.60 |
| 67 | 5 | 5004 | C | N3-C4-N4 | 9.95 | 124.97 | 118.00 |
| 67 | 5 | 51 | A | N1-C6-N6 | 9.92 | 124.55 | 118.60 |
| 67 | 5 | 1191 | C | C6-N1-C2 | -9.92 | 116.33 | 120.30 |
| 67 | 5 | 4980 | C | C5-C4-N4 | -9.89 | 113.27 | 120.20 |
| 76 | 9 | 876 | C | N1-C2-O2 | 9.87 | 124.82 | 118.90 |
| 67 | 5 | 4378 | A | O4'-C1'-N9 | 9.80 | 116.04 | 108.20 |
| 67 | 5 | 64 | A | N1-C6-N6 | 9.78 | 124.47 | 118.60 |
| 67 | 5 | 4533 | A | N1-C6-N6 | 9.77 | 124.46 | 118.60 |
| 67 | 5 | 4723 | A | C5-C6-N1 | 9.72 | 122.56 | 117.70 |
| 67 | 5 | 1580 | C | C2-N1-C1' | 9.72 | 129.49 | 118.80 |
| 67 | 5 | 106 | A | N1-C6-N6 | 9.70 | 124.42 | 118.60 |
| 67 | 5 | 3911 | C | C2-N1-C1' | 9.69 | 129.45 | 118.80 |
| 67 | 5 | 294 | G | C8-N9-C1' | -9.67 | 114.43 | 127.00 |
| 67 | 5 | 39 | A | C8-N9-C4 | -9.67 | 101.93 | 105.80 |
| 67 | 5 | 64 | A | C5-C6-N6 | -9.65 | 115.98 | 123.70 |
| 67 | 5 | 1587 | G | C8-N9-C4 | -9.64 | 102.54 | 106.40 |
| 67 | 5 | 2068 | C | C5-C4-N4 | -9.59 | 113.49 | 120.20 |
| 67 | 5 | 38 | A | C6-C5-N7 | -9.58 | 125.60 | 132.30 |
| 67 | 5 | 1680 | G | N1-C2-N2 | -9.58 | 107.58 | 116.20 |
| 67 | 5 | 3860 | A | N1-C6-N6 | -9.52 | 112.89 | 118.60 |
| 76 | 9 | 1513 | C | N3-C2-O2 | -9.51 | 115.25 | 121.90 |
| 76 | 9 | 1458 | G | O5'-P-OP1 | -9.50 | 97.15 | 105.70 |
| 76 | 9 | 52 | G | N3-C4-C5 | 9.47 | 133.33 | 128.60 |
| 67 | 5 | 1898 | C | C5-C4-N4 | -9.45 | 113.59 | 120.20 |
| 67 | 5 | 50 | C | C5-C4-N4 | -9.44 | 113.59 | 120.20 |
| 67 | 5 | 1065 | G | N3-C4-N9 | -9.42 | 120.35 | 126.00 |
| 67 | 5 | 3653 | A | C4-N9-C1' | 9.36 | 143.14 | 126.30 |
| 67 | 5 | 2025 | A | C5-C6-N1 | 9.35 | 122.37 | 117.70 |
| 67 | 5 | 1541 | C | C2-N1-C1' | 9.35 | 129.08 | 118.80 |
| 67 | 5 | 39 | A | C8-N9-C1' | -9.34 | 110.90 | 127.70 |
| 67 | 5 | 4279 | A | N1-C6-N6 | 9.30 | 124.18 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4528 | G | C8-N9-C4 | -9.29 | 102.68 | 106.40 |
| 67 | 5 | 5016 | A | N1-C6-N6 | 9.24 | 124.14 | 118.60 |
| 67 | 5 | 4536 | C | N1-C2-O2 | 9.20 | 124.42 | 118.90 |
| 76 | 9 | 672 | A | O4'-C1'-N9 | 9.16 | 115.53 | 108.20 |
| 67 | 5 | 1521 | C | C5-C4-N4 | -9.15 | 113.79 | 120.20 |
| 67 | 5 | 2815 | A | C5-C6-N6 | -9.15 | 116.38 | 123.70 |
| 67 | 5 | 1507 | C | C6-N1-C2 | -9.13 | 116.65 | 120.30 |
| 67 | 5 | 299 | C | N1-C2-O2 | 9.09 | 124.35 | 118.90 |
| 67 | 5 | 1535 | C | N3-C4-C5 | 9.08 | 125.53 | 121.90 |
| 67 | 5 | 1674 | C | N1-C2-O2 | 9.08 | 124.35 | 118.90 |
| 67 | 5 | 1076 | C | N3-C2-O2 | -9.08 | 115.54 | 121.90 |
| 67 | 5 | 90 | G | C8-N9-C4 | -9.06 | 102.78 | 106.40 |
| 67 | 5 | 2799 | G | C8-N9-C1' | -9.06 | 115.23 | 127.00 |
| 67 | 5 | 2540 | C | C6-N1-C2 | -9.04 | 116.68 | 120.30 |
| 76 | 9 | 140 | U | C6-N1-C2 | -9.04 | 115.58 | 121.00 |
| 67 | 5 | 1675 | C | N3-C2-O2 | -9.00 | 115.60 | 121.90 |
| 76 | 9 | 524 | U | C5-C4-O4 | -8.98 | 120.51 | 125.90 |
| 76 | 9 | 1245 | G | N3-C4-C5 | -8.96 | 124.12 | 128.60 |
| 8 | EE | 48 | LEU | CB-CG-CD1 | 8.95 | 126.22 | 111.00 |
| 67 | 5 | 2078 | C | C2-N1-C1' | 8.95 | 128.65 | 118.80 |
| 76 | 9 | 1096 | G | N3-C2-N2 | 8.90 | 126.13 | 119.90 |
| 67 | 5 | 1928 | C | C6-N1-C2 | 8.89 | 123.86 | 120.30 |
| 67 | 5 | 1651 | G | N1-C2-N2 | -8.86 | 108.23 | 116.20 |
| 67 | 5 | 3650 | C | C2-N1-C1' | 8.86 | 128.55 | 118.80 |
| 76 | 9 | 1563 | G | N3-C4-C5 | 8.85 | 133.02 | 128.60 |
| 67 | 5 | 3749 | C | C2-N1-C1' | 8.83 | 128.52 | 118.80 |
| 67 | 5 | 1623 | A | N1-C6-N6 | 8.82 | 123.89 | 118.60 |
| 67 | 5 | 2410 | C | C2-N1-C1' | 8.79 | 128.47 | 118.80 |
| 67 | 5 | 2833 | A | O4'-C1'-N9 | 8.79 | 115.23 | 108.20 |
| 67 | 5 | 1081 | C | C6-N1-C1' | -8.79 | 110.26 | 120.80 |
| 67 | 5 | 1580 | C | C6-N1-C2 | -8.78 | 116.79 | 120.30 |
| 67 | 5 | 1632 | A | C8-N9-C4 | -8.75 | 102.30 | 105.80 |
| 67 | 5 | 1938 | C | C6-N1-C2 | 8.73 | 123.79 | 120.30 |
| 67 | 5 | 2465 | C | C2-N1-C1' | 8.69 | 128.35 | 118.80 |
| 67 | 5 | 1648 | C | N1-C2-O2 | 8.68 | 124.11 | 118.90 |
| 67 | 5 | 2815 | A | C4-C5-N7 | 8.68 | 115.04 | 110.70 |
| 67 | 5 | 2346 | C | O4'-C1'-N1 | 8.65 | 115.12 | 108.20 |
| 67 | 5 | 4971 | A | N1-C6-N6 | -8.65 | 113.41 | 118.60 |
| 67 | 5 | 3882 | C | C6-N1-C2 | -8.64 | 116.84 | 120.30 |
| 76 | 9 | 1490 | G | N3-C4-C5 | -8.63 | 124.28 | 128.60 |
| 67 | 5 | 3774 | A | N1-C6-N6 | 8.63 | 123.78 | 118.60 |
| 67 | 5 | 356 | G | C2-N3-C4 | -8.63 | 107.59 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1851 | G | C4-N9-C1' | 8.62 | 137.71 | 126.50 |
| 67 | 5 | 3876 | A | N1-C6-N6 | -8.62 | 113.43 | 118.60 |
| 76 | 9 | 1513 | C | N1-C2-O2 | 8.60 | 124.06 | 118.90 |
| 67 | 5 | 1648 | C | N3-C2-O2 | -8.59 | 115.88 | 121.90 |
| 67 | 5 | 355 | A | C5-C6-N6 | -8.58 | 116.83 | 123.70 |
| 67 | 5 | 2393 | C | C5-C4-N4 | -8.57 | 114.20 | 120.20 |
| 76 | 9 | 1254 | C | O4'-C1'-N1 | 8.57 | 115.05 | 108.20 |
| 67 | 5 | 1465 | G | C4-N9-C1' | 8.56 | 137.63 | 126.50 |
| 67 | 5 | 1928 | C | N3-C4-C5 | 8.55 | 125.32 | 121.90 |
| 67 | 5 | 3917 | A | C5-C6-N6 | -8.53 | 116.88 | 123.70 |
| 73 | 8 | 103 | A | C6-C5-N7 | -8.52 | 126.33 | 132.30 |
| 67 | 5 | 1318 | C | C5-C4-N4 | -8.50 | 114.25 | 120.20 |
| 76 | 9 | 1096 | G | N1-C2-N2 | -8.50 | 108.55 | 116.20 |
| 67 | 5 | 3945 | A | P-O3'-C3' | 8.50 | 129.90 | 119.70 |
| 82 | c | 20 | LEU | CA-CB-CG | 8.49 | 134.82 | 115.30 |
| 67 | 5 | 1941 | A | N1-C6-N6 | -8.49 | 113.51 | 118.60 |
| 67 | 5 | 2410 | C | C6-N1-C1' | -8.48 | 110.63 | 120.80 |
| 76 | 9 | 1532 | C | C2-N1-C1' | 8.46 | 128.11 | 118.80 |
| 67 | 5 | 3909 | C | C6-N1-C2 | 8.45 | 123.68 | 120.30 |
| 67 | 5 | 1872 | G | C2-N3-C4 | -8.45 | 107.68 | 111.90 |
| 76 | 9 | 1658 | G | C4-C5-N7 | 8.45 | 114.18 | 110.80 |
| 76 | 9 | 524 | U | N3-C4-O4 | 8.43 | 125.30 | 119.40 |
| 76 | 9 | 1416 | C | C2-N1-C1' | 8.43 | 128.07 | 118.80 |
| 76 | 9 | 1562 | C | C6-N1-C2 | 8.41 | 123.66 | 120.30 |
| 67 | 5 | 4533 | A | C5-C6-N6 | -8.41 | 116.97 | 123.70 |
| 67 | 5 | 5016 | A | C5-C6-N6 | -8.40 | 116.98 | 123.70 |
| 67 | 5 | 1680 | G | N3-C2-N2 | 8.39 | 125.78 | 119.90 |
| 67 | 5 | 1065 | G | N3-C4-C5 | 8.39 | 132.79 | 128.60 |
| 67 | 5 | 4618 | G | C8-N9-C4 | -8.35 | 103.06 | 106.40 |
| 67 | 5 | 4463 | U | O4'-C1'-N1 | 8.35 | 114.88 | 108.20 |
| 67 | 5 | 4193 | C | C2-N1-C1' | 8.34 | 127.97 | 118.80 |
| 76 | 9 | 1495 | G | O4'-C1'-N9 | -8.34 | 101.53 | 108.20 |
| 67 | 5 | 1675 | C | C6-N1-C2 | -8.33 | 116.97 | 120.30 |
| 76 | 9 | 1603 | G | C8-N9-C1' | -8.32 | 116.19 | 127.00 |
| 67 | 5 | 968 | C | N1-C2-O2 | 8.31 | 123.89 | 118.90 |
| 76 | 9 | 1219 | C | C2-N1-C1' | 8.31 | 127.94 | 118.80 |
| 67 | 5 | 3910 | C | C2-N1-C1' | 8.30 | 127.93 | 118.80 |
| 67 | 5 | 1515 | A | C5-C6-N1 | 8.28 | 121.84 | 117.70 |
| 76 | 9 | 1218 | C | C6-N1-C2 | -8.26 | 116.99 | 120.30 |
| 76 | 9 | 1638 | G | P-O3'-C3' | 8.25 | 129.60 | 119.70 |
| 67 | 5 | 1675 | C | N1-C2-O2 | 8.25 | 123.85 | 118.90 |
| 76 | 9 | 1490 | G | N3-C4-N9 | 8.24 | 130.95 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4448 | G | C2-N3-C4 | -8.24 | 107.78 | 111.90 |
| 76 | 9 | 909 | G | N3-C4-N9 | 8.23 | 130.94 | 126.00 |
| 67 | 5 | 3774 | A | C5-C6-N6 | -8.22 | 117.12 | 123.70 |
| 67 | 5 | 3737 | A | N1-C6-N6 | 8.20 | 123.52 | 118.60 |
| 67 | 5 | 2527 | A | N1-C6-N6 | -8.19 | 113.68 | 118.60 |
| 67 | 5 | 143 | C | C6-N1-C2 | -8.15 | 117.04 | 120.30 |
| 76 | 9 | 1019 | C | C6-N1-C2 | -8.15 | 117.04 | 120.30 |
| 67 | 5 | 38 | A | N9-C4-C5 | -8.14 | 102.54 | 105.80 |
| 67 | 5 | 2815 | A | N1-C6-N6 | 8.14 | 123.48 | 118.60 |
| 67 | 5 | 159 | C | C2-N1-C1' | 8.13 | 127.75 | 118.80 |
| 67 | 5 | 4626 | A | N1-C6-N6 | -8.13 | 113.72 | 118.60 |
| 67 | 5 | 3749 | C | C6-N1-C2 | -8.11 | 117.06 | 120.30 |
| 76 | 9 | 1658 | G | C6-C5-N7 | -8.11 | 125.53 | 130.40 |
| 67 | 5 | 978 | G | O4'-C1'-N9 | 8.10 | 114.68 | 108.20 |
| 67 | 5 | 384 | A | N1-C6-N6 | -8.09 | 113.75 | 118.60 |
| 76 | 9 | 1563 | G | C8-N9-C4 | 8.08 | 109.63 | 106.40 |
| 67 | 5 | 294 | G | C4-N9-C1' | 8.07 | 137.00 | 126.50 |
| 76 | 9 | 1603 | G | C4-N9-C1' | 8.07 | 136.99 | 126.50 |
| 67 | 5 | 1812 | C | C6-N1-C1' | -8.07 | 111.12 | 120.80 |
| 67 | 5 | 159 | C | N3-C4-N4 | 8.06 | 123.64 | 118.00 |
| 67 | 5 | 1924 | C | N1-C2-O2 | 8.06 | 123.73 | 118.90 |
| 67 | 5 | 2499 | C | N3-C2-O2 | -8.05 | 116.27 | 121.90 |
| 67 | 5 | 1675 | C | C2-N1-C1' | 8.05 | 127.65 | 118.80 |
| 67 | 5 | 1191 | C | N3-C2-O2 | -8.03 | 116.28 | 121.90 |
| 76 | 9 | 347 | G | N3-C2-N2 | -8.02 | 114.28 | 119.90 |
| 67 | 5 | 1515 | A | C6-N1-C2 | -8.01 | 113.79 | 118.60 |
| 67 | 5 | 1851 | G | C8-N9-C1' | -8.01 | 116.58 | 127.00 |
| 76 | 9 | 1305 | C | N3-C2-O2 | -8.01 | 116.29 | 121.90 |
| 67 | 5 | 4723 | A | N1-C2-N3 | 8.00 | 133.30 | 129.30 |
| 67 | 5 | 30 | C | N3-C2-O2 | -7.99 | 116.31 | 121.90 |
| 67 | 5 | 1662 | C | C2-N1-C1' | 7.99 | 127.58 | 118.80 |
| 67 | 5 | 1674 | C | N3-C2-O2 | -7.99 | 116.31 | 121.90 |
| 67 | 5 | 1986 | U | P-O3'-C3' | 7.97 | 129.27 | 119.70 |
| 67 | 5 | 3749 | C | N3-C2-O2 | -7.97 | 116.32 | 121.90 |
| 67 | 5 | 1662 | C | N1-C2-O2 | 7.97 | 123.68 | 118.90 |
| 67 | 5 | 1653 | A | N9-C4-C5 | -7.97 | 102.61 | 105.80 |
| 67 | 5 | 352 | G | O4'-C1'-N9 | -7.96 | 101.83 | 108.20 |
| 67 | 5 | 2411 | C | C2-N1-C1' | 7.95 | 127.54 | 118.80 |
| 67 | 5 | 2509 | C | C2-N1-C1' | 7.94 | 127.53 | 118.80 |
| 67 | 5 | 3917 | A | C6-N1-C2 | -7.93 | 113.84 | 118.60 |
| 67 | 5 | 1577 | G | O4'-C1'-N9 | 7.91 | 114.53 | 108.20 |
| 67 | 5 | 1651 | G | C4-N9-C1' | 7.90 | 136.78 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 3910 | C | N3-C2-O2 | -7.89 | 116.37 | 121.90 |
| 67 | 5 | 2671 | C | N3-C2-O2 | -7.89 | 116.38 | 121.90 |
| 67 | 5 | 956 | A | N1-C6-N6 | -7.88 | 113.87 | 118.60 |
| 67 | 5 | 1501 | C | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 67 | 5 | 4338 | G | C2-N3-C4 | -7.87 | 107.97 | 111.90 |
| 67 | 5 | 2274 | C | C6-N1-C2 | -7.85 | 117.16 | 120.30 |
| 67 | 5 | 2670 | C | N1-C2-O2 | 7.84 | 123.61 | 118.90 |
| 67 | 5 | 1847 | C | C2-N1-C1' | 7.82 | 127.41 | 118.80 |
| 67 | 5 | 1651 | G | C6-C5-N7 | -7.81 | 125.71 | 130.40 |
| 76 | 9 | 909 | G | N3-C4-C5 | -7.81 | 124.70 | 128.60 |
| 67 | 5 | 2860 | C | N3-C4-N4 | 7.80 | 123.46 | 118.00 |
| 67 | 5 | 1465 | G | C8-N9-C1' | -7.78 | 116.89 | 127.00 |
| 67 | 5 | 3774 | A | N9-C4-C5 | -7.78 | 102.69 | 105.80 |
| 67 | 5 | 302 | C | N1-C2-O2 | 7.77 | 123.56 | 118.90 |
| 67 | 5 | 4555 | U | O4'-C1'-N1 | 7.77 | 114.42 | 108.20 |
| 67 | 5 | 1327 | C | N1-C2-O2 | 7.76 | 123.56 | 118.90 |
| 67 | 5 | 38 | A | C5-C6-N6 | -7.75 | 117.50 | 123.70 |
| 67 | 5 | 1794 | A | C8-N9-C4 | -7.75 | 102.70 | 105.80 |
| 67 | 5 | 2299 | G | C8-N9-C4 | -7.75 | 103.30 | 106.40 |
| 67 | 5 | 3650 | C | C5-C4-N4 | -7.74 | 114.78 | 120.20 |
| 67 | 5 | 106 | A | C8-N9-C1' | -7.74 | 113.77 | 127.70 |
| 4 | DD | 29 | LEU | CB-CG-CD2 | -7.73 | 97.86 | 111.00 |
| 67 | 5 | 4279 | A | C5-C6-N6 | -7.73 | 117.52 | 123.70 |
| 67 | 5 | 4214 | A | C5-C6-N1 | 7.73 | 121.56 | 117.70 |
| 67 | 5 | 1323 | A | C5-C6-N6 | -7.71 | 117.53 | 123.70 |
| 67 | 5 | 2802 | C | N3-C2-O2 | -7.71 | 116.50 | 121.90 |
| 67 | 5 | 159 | C | C6-N1-C1' | -7.71 | 111.55 | 120.80 |
| 67 | 5 | 2337 | C | C6-N1-C2 | -7.71 | 117.22 | 120.30 |
| 67 | 5 | 4362 | A | C8-N9-C4 | -7.71 | 102.72 | 105.80 |
| 76 | 9 | 1019 | C | C2-N1-C1' | 7.70 | 127.27 | 118.80 |
| 67 | 5 | 4654 | C | N1-C2-O2 | 7.69 | 123.52 | 118.90 |
| 67 | 5 | 955 | G | N1-C2-N2 | -7.68 | 109.29 | 116.20 |
| 67 | 5 | 2068 | C | N3-C4-N4 | 7.67 | 123.37 | 118.00 |
| 67 | 5 | 2781 | G | C8-N9-C1' | -7.67 | 117.02 | 127.00 |
| 67 | 5 | 1868 | A | N1-C6-N6 | 7.67 | 123.20 | 118.60 |
| 67 | 5 | 2579 | G | N3-C4-C5 | 7.67 | 132.44 | 128.60 |
| 76 | 9 | 350 | C | C5-C4-N4 | -7.66 | 114.84 | 120.20 |
| 67 | 5 | 2853 | C | C6-N1-C2 | 7.66 | 123.36 | 120.30 |
| 67 | 5 | 1646 | A | C6-N1-C2 | -7.65 | 114.01 | 118.60 |
| 67 | 5 | 727 | C | C6-N1-C2 | -7.64 | 117.24 | 120.30 |
| 67 | 5 | 1651 | G | C8-N9-C1' | -7.64 | 117.06 | 127.00 |
| 67 | 5 | 1682 | A | C6-N1-C2 | -7.64 | 114.02 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 50 | C | N3-C4-C5 | 7.64 | 124.95 | 121.90 |
| 67 | 5 | 1327 | C | C2-N1-C1' | 7.62 | 127.19 | 118.80 |
| 67 | 5 | 2465 | C | C6-N1-C1' | -7.62 | 111.65 | 120.80 |
| 67 | 5 | 2291 | G | C2-N3-C4 | -7.62 | 108.09 | 111.90 |
| 67 | 5 | 4654 | C | C2-N1-C1' | 7.61 | 127.17 | 118.80 |
| 76 | 9 | 1055 | A | N1-C6-N6 | 7.61 | 123.16 | 118.60 |
| 67 | 5 | 2025 | A | C5-C6-N6 | -7.60 | 117.62 | 123.70 |
| 67 | 5 | 3866 | C | C2-N1-C1' | 7.60 | 127.16 | 118.80 |
| 67 | 5 | 1870 | C | N3-C4-C5 | 7.58 | 124.93 | 121.90 |
| 67 | 5 | 106 | A | C4-N9-C1' | 7.58 | 139.95 | 126.30 |
| 76 | 9 | 1219 | C | C5-C6-N1 | 7.58 | 124.79 | 121.00 |
| 67 | 5 | 1191 | C | O4'-C1'-N1 | 7.57 | 114.26 | 108.20 |
| 67 | 5 | 1576 | G | C8-N9-C1' | -7.57 | 117.16 | 127.00 |
| 67 | 5 | 2093 | G | O4'-C1'-N9 | 7.57 | 114.25 | 108.20 |
| 67 | 5 | 3871 | A | C6-N1-C2 | -7.57 | 114.06 | 118.60 |
| 67 | 5 | 2785 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 67 | 5 | 299 | C | N3-C2-O2 | -7.56 | 116.61 | 121.90 |
| 67 | 5 | 2815 | A | N9-C4-C5 | -7.56 | 102.78 | 105.80 |
| 76 | 9 | 319 | C | C2-N1-C1' | -7.55 | 110.49 | 118.80 |
| 67 | 5 | 3911 | C | N3-C2-O2 | -7.55 | 116.61 | 121.90 |
| 67 | 5 | 1357 | C | N1-C2-O2 | 7.55 | 123.43 | 118.90 |
| 73 | 8 | 15 | G | C2-N3-C4 | -7.55 | 108.12 | 111.90 |
| 67 | 5 | 83 | C | N3-C4-C5 | 7.55 | 124.92 | 121.90 |
| 67 | 5 | 292 | G | C8-N9-C1' | -7.55 | 117.19 | 127.00 |
| 67 | 5 | 38 | A | C4-C5-N7 | 7.54 | 114.47 | 110.70 |
| 67 | 5 | 38 | A | C8-N9-C1' | -7.54 | 114.13 | 127.70 |
| 67 | 5 | 2277 | C | N1-C2-O2 | 7.53 | 123.42 | 118.90 |
| 67 | 5 | 3749 | C | N1-C2-O2 | 7.53 | 123.42 | 118.90 |
| 70 | 7 | 11 | A | C8-N9-C4 | 7.53 | 108.81 | 105.80 |
| 67 | 5 | 1323 | A | N1-C6-N6 | 7.52 | 123.11 | 118.60 |
| 67 | 5 | 4583 | C | O4'-C1'-N1 | 7.52 | 114.21 | 108.20 |
| 67 | 5 | 1931 | C | C2-N1-C1' | 7.51 | 127.07 | 118.80 |
| 67 | 5 | 106 | A | C6-C5-N7 | -7.51 | 127.04 | 132.30 |
| 67 | 5 | 39 | A | C4-N9-C1' | 7.51 | 139.81 | 126.30 |
| 67 | 5 | 51 | A | C6-C5-N7 | -7.51 | 127.05 | 132.30 |
| 76 | 9 | 1825 | A | O4'-C1'-N9 | 7.50 | 114.20 | 108.20 |
| 67 | 5 | 64 | A | N9-C4-C5 | -7.50 | 102.80 | 105.80 |
| 67 | 5 | 2781 | G | C4-N9-C1' | 7.50 | 136.24 | 126.50 |
| 67 | 5 | 106 | A | O4'-C1'-N9 | -7.49 | 102.21 | 108.20 |
| 67 | 5 | 332 | C | N3-C4-C5 | 7.49 | 124.89 | 121.90 |
| 73 | 8 | 44 | A | C5-C6-N6 | -7.49 | 117.71 | 123.70 |
| 67 | 5 | 292 | G | C4-N9-C1' | 7.48 | 136.22 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1357 | C | C2-N1-C1' | 7.48 | 127.02 | 118.80 |
| 67 | 5 | 2335 | C | N1-C2-O2 | 7.47 | 123.38 | 118.90 |
| 67 | 5 | 4688 | C | C5-C4-N4 | -7.47 | 114.97 | 120.20 |
| 67 | 5 | 1674 | C | C5-C4-N4 | -7.47 | 114.97 | 120.20 |
| 76 | 9 | 1250 | A | O4'-C1'-N9 | -7.46 | 102.23 | 108.20 |
| 76 | 9 | 1715 | A | N1-C6-N6 | 7.46 | 123.08 | 118.60 |
| 67 | 5 | 293 | G | C8-N9-C1' | -7.46 | 117.31 | 127.00 |
| 67 | 5 | 1599 | G | N1-C2-N2 | -7.46 | 109.49 | 116.20 |
| 67 | 5 | 1589 | C | N1-C2-O2 | 7.45 | 123.37 | 118.90 |
| 67 | 5 | 2078 | C | C6-N1-C1' | -7.45 | 111.87 | 120.80 |
| 67 | 5 | 2319 | C | C5-C4-N4 | -7.43 | 115.00 | 120.20 |
| 67 | 5 | 1235 | G | N3-C4-N9 | -7.43 | 121.54 | 126.00 |
| 67 | 5 | 1879 | C | C5-C4-N4 | -7.43 | 115.00 | 120.20 |
| 67 | 5 | 384 | A | O4'-C1'-N9 | 7.41 | 114.13 | 108.20 |
| 67 | 5 | 1327 | C | C5-C4-N4 | -7.41 | 115.02 | 120.20 |
| 67 | 5 | 39 | A | N1-C6-N6 | 7.40 | 123.04 | 118.60 |
| 67 | 5 | 408 | A | C8-N9-C4 | -7.40 | 102.84 | 105.80 |
| 67 | 5 | 2815 | A | C6-C5-N7 | -7.39 | 127.13 | 132.30 |
| 67 | 5 | 1670 | G | N3-C2-N2 | 7.39 | 125.07 | 119.90 |
| 76 | 9 | 998 | A | O4'-C1'-N9 | 7.38 | 114.11 | 108.20 |
| 67 | 5 | 264 | C | C5-C4-N4 | -7.38 | 115.03 | 120.20 |
| 67 | 5 | 38 | A | C4-N9-C1' | 7.36 | 139.55 | 126.30 |
| 73 | 8 | 15 | G | C8-N9-C1' | -7.36 | 117.43 | 127.00 |
| 67 | 5 | 3774 | A | C8-N9-C1' | -7.36 | 114.46 | 127.70 |
| 67 | 5 | 3887 | C | C6-N1-C2 | 7.36 | 123.24 | 120.30 |
| 67 | 5 | 2039 | G | C8-N9-C1' | -7.35 | 117.44 | 127.00 |
| 73 | 8 | 44 | A | N1-C6-N6 | 7.35 | 123.01 | 118.60 |
| 76 | 9 | 1849 | G | C4-N9-C1' | 7.35 | 136.06 | 126.50 |
| 67 | 5 | 112 | C | C2-N1-C1' | 7.34 | 126.88 | 118.80 |
| 67 | 5 | 3771 | C | C2-N1-C1' | 7.34 | 126.88 | 118.80 |
| 70 | 7 | 36 | C | N1-C2-O2 | 7.34 | 123.30 | 118.90 |
| 76 | 9 | 1245 | G | N3-C4-N9 | 7.33 | 130.40 | 126.00 |
| 67 | 5 | 38 | A | O4'-C1'-N9 | -7.33 | 102.34 | 108.20 |
| 67 | 5 | 2025 | A | C8-N9-C4 | 7.33 | 108.73 | 105.80 |
| 67 | 5 | 4603 | C | C2-N1-C1' | 7.32 | 126.85 | 118.80 |
| 67 | 5 | 332 | C | C5-C4-N4 | -7.32 | 115.08 | 120.20 |
| 76 | 9 | 350 | C | N3-C4-C5 | 7.31 | 124.83 | 121.90 |
| 22 | HH | 72 | PHE | CB-CG-CD2 | -7.31 | 115.68 | 120.80 |
| 67 | 5 | 671 | G | N3-C4-N9 | -7.30 | 121.62 | 126.00 |
| 76 | 9 | 1216 | C | N3-C4-N4 | -7.29 | 112.89 | 118.00 |
| 67 | 5 | 303 | C | N3-C2-O2 | -7.29 | 116.80 | 121.90 |
| 67 | 5 | 3916 | G | N3-C4-C5 | -7.29 | 124.96 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 386 | A | N1-C6-N6 | 7.29 | 122.97 | 118.60 |
| 76 | 9 | 603 | C | N3-C4-C5 | 7.29 | 124.81 | 121.90 |
| 67 | 5 | 1456 | C | N3-C4-C5 | 7.27 | 124.81 | 121.90 |
| 67 | 5 | 4215 | C | N3-C4-C5 | 7.27 | 124.81 | 121.90 |
| 33 | J | 63 | ARG | NE-CZ-NH2 | -7.27 | 116.66 | 120.30 |
| 67 | 5 | 2003 | G | O5'-P-OP2 | -7.27 | 99.16 | 105.70 |
| 67 | 5 | 4717 | A | C5-C6-N6 | -7.27 | 117.88 | 123.70 |
| 76 | 9 | 876 | C | N3-C2-O2 | -7.27 | 116.81 | 121.90 |
| 67 | 5 | 1864 | G | N3-C4-C5 | -7.27 | 124.97 | 128.60 |
| 67 | 5 | 1665 | C | N1-C2-O2 | 7.26 | 123.26 | 118.90 |
| 67 | 5 | 4331 | G | N1-C2-N2 | -7.26 | 109.66 | 116.20 |
| 67 | 5 | 1580 | C | N3-C2-O2 | -7.26 | 116.82 | 121.90 |
| 67 | 5 | 356 | G | N1-C2-N2 | -7.26 | 109.67 | 116.20 |
| 67 | 5 | 1580 | C | C6-N1-C1' | -7.26 | 112.09 | 120.80 |
| 67 | 5 | 2785 | C | C6-N1-C1' | -7.26 | 112.09 | 120.80 |
| 67 | 5 | 81 | C | N1-C2-O2 | 7.26 | 123.25 | 118.90 |
| 32 | jj | 353 | LEU | CB-CG-CD2 | 7.26 | 123.34 | 111.00 |
| 67 | 5 | 2024 | G | N3-C4-N9 | -7.26 | 121.65 | 126.00 |
| 67 | 5 | 386 | A | C6-C5-N7 | -7.25 | 127.22 | 132.30 |
| 67 | 5 | 4525 | C | N1-C2-O2 | 7.25 | 123.25 | 118.90 |
| 76 | 9 | 363 | A | O4'-C1'-N9 | 7.25 | 114.00 | 108.20 |
| 67 | 5 | 1235 | G | C2-N3-C4 | -7.25 | 108.28 | 111.90 |
| 67 | 5 | 1081 | C | C5-C6-N1 | 7.25 | 124.62 | 121.00 |
| 67 | 5 | 4868 | G | N3-C4-C5 | -7.25 | 124.98 | 128.60 |
| 67 | 5 | 3748 | A | C6-N1-C2 | -7.24 | 114.25 | 118.60 |
| 67 | 5 | 747 | A | N1-C6-N6 | 7.24 | 122.94 | 118.60 |
| 67 | 5 | 2411 | C | C6-N1-C1' | -7.24 | 112.11 | 120.80 |
| 73 | 8 | 26 | C | C5-C4-N4 | -7.24 | 115.13 | 120.20 |
| 67 | 5 | 1868 | A | C8-N9-C4 | -7.24 | 102.90 | 105.80 |
| 67 | 5 | 2731 | C | N1-C2-O2 | 7.24 | 123.24 | 118.90 |
| 76 | 9 | 1811 | C | N1-C2-O2 | 7.23 | 123.24 | 118.90 |
| 67 | 5 | 1327 | C | C6-N1-C1' | -7.22 | 112.14 | 120.80 |
| 67 | 5 | 1646 | A | N1-C2-N3 | 7.21 | 132.91 | 129.30 |
| 67 | 5 | 80 | C | N1-C2-O2 | 7.21 | 123.22 | 118.90 |
| 67 | 5 | 1892 | A | C5-C6-N1 | 7.20 | 121.30 | 117.70 |
| 28 | ii | 189 | ARG | CG-CD-NE | 7.20 | 126.92 | 111.80 |
| 67 | 5 | 1534 | A | O4'-C1'-N9 | 7.20 | 113.96 | 108.20 |
| 67 | 5 | 3919 | C | C6-N1-C2 | -7.20 | 117.42 | 120.30 |
| 67 | 5 | 2499 | C | N1-C2-O2 | 7.20 | 123.22 | 118.90 |
| 76 | 9 | 1216 | C | O4'-C1'-N1 | 7.19 | 113.95 | 108.20 |
| 67 | 5 | 218 | A | O4'-C1'-N9 | -7.19 | 102.45 | 108.20 |
| 67 | 5 | 1427 | A | N1-C6-N6 | 7.19 | 122.91 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1535 | C | N3-C4-N4 | 7.18 | 123.03 | 118.00 |
| 67 | 5 | 1653 | A | C6-C5-N7 | -7.18 | 127.27 | 132.30 |
| 67 | 5 | 4179 | G | C4-N9-C1' | 7.18 | 135.83 | 126.50 |
| 76 | 9 | 813 | A | O5'-P-OP1 | -7.18 | 99.24 | 105.70 |
| 76 | 9 | 347 | G | N3-C4-N9 | -7.17 | 121.69 | 126.00 |
| 67 | 5 | 4911 | A | O4'-C1'-N9 | -7.17 | 102.47 | 108.20 |
| 76 | 9 | 1438 | A | C5-C6-N6 | -7.17 | 117.97 | 123.70 |
| 73 | 8 | 79 | G | C4-N9-C1' | 7.16 | 135.81 | 126.50 |
| 67 | 5 | 2458 | C | N1-C2-O2 | 7.16 | 123.19 | 118.90 |
| 67 | 5 | 4971 | A | O4'-C1'-N9 | 7.16 | 113.93 | 108.20 |
| 73 | 8 | 103 | A | C5-C6-N6 | -7.16 | 117.97 | 123.70 |
| 67 | 5 | 351 | C | C2-N1-C1' | 7.15 | 126.67 | 118.80 |
| 67 | 5 | 1343 | A | C6-N1-C2 | -7.15 | 114.31 | 118.60 |
| 67 | 5 | 5004 | C | C2-N1-C1' | 7.14 | 126.66 | 118.80 |
| 67 | 5 | 2815 | A | C5-N7-C8 | -7.14 | 100.33 | 103.90 |
| 67 | 5 | 1191 | C | C6-N1-C1' | 7.13 | 129.36 | 120.80 |
| 67 | 5 | 4513 | A | C5-C6-N6 | -7.13 | 118.00 | 123.70 |
| 67 | 5 | 2397 | G | N1-C2-N2 | -7.12 | 109.79 | 116.20 |
| 67 | 5 | 3845 | A | C6-N1-C2 | -7.12 | 114.33 | 118.60 |
| 67 | 5 | 2078 | C | C6-N1-C2 | -7.12 | 117.45 | 120.30 |
| 76 | 9 | 826 | A | N1-C6-N6 | -7.11 | 114.33 | 118.60 |
| 67 | 5 | 159 | C | C5-C4-N4 | -7.11 | 115.22 | 120.20 |
| 67 | 5 | 2850 | A | C6-N1-C2 | -7.11 | 114.34 | 118.60 |
| 67 | 5 | 4166 | G | N3-C2-N2 | 7.11 | 124.87 | 119.90 |
| 67 | 5 | 1306 | C | C2-N1-C1' | 7.10 | 126.61 | 118.80 |
| 67 | 5 | 4456 | C | N3-C2-O2 | -7.10 | 116.93 | 121.90 |
| 67 | 5 | 2802 | C | N1-C2-O2 | 7.09 | 123.16 | 118.90 |
| 67 | 5 | 4087 | G | N3-C4-N9 | -7.09 | 121.74 | 126.00 |
| 76 | 9 | 4 | C | N3-C4-C5 | 7.09 | 124.74 | 121.90 |
| 17 | BB | 113 | MET | CG-SD-CE | -7.09 | 88.86 | 100.20 |
| 67 | 5 | 4645 | C | N1-C2-O2 | 7.08 | 123.15 | 118.90 |
| 76 | 9 | 329 | G | C4-N9-C1' | 7.08 | 135.70 | 126.50 |
| 32 | jj | 384 | LYS | CB-CG-CD | 7.07 | 129.99 | 111.60 |
| 67 | 5 | 1938 | C | N3-C4-C5 | 7.07 | 124.73 | 121.90 |
| 67 | 5 | 11 | G | C4-N9-C1' | 7.06 | 135.68 | 126.50 |
| 67 | 5 | 2381 | A | N1-C6-N6 | -7.06 | 114.36 | 118.60 |
| 22 | HH | 72 | PHE | CB-CG-CD1 | 7.06 | 125.74 | 120.80 |
| 67 | 5 | 351 | C | C6-N1-C2 | -7.05 | 117.48 | 120.30 |
| 67 | 5 | 356 | G | N1-C2-N3 | 7.05 | 128.13 | 123.90 |
| 67 | 5 | 1859 | C | C5-C4-N4 | -7.05 | 115.26 | 120.20 |
| 73 | 8 | 19 | C | N1-C2-O2 | 7.05 | 123.13 | 118.90 |
| 67 | 5 | 1357 | C | C6-N1-C1' | -7.05 | 112.34 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1674 | C | C2-N1-C1' | 7.04 | 126.55 | 118.80 |
| 67 | 5 | 4945 | G | C8-N9-C1' | -7.04 | 117.84 | 127.00 |
| 67 | 5 | 1794 | A | N7-C8-N9 | 7.04 | 117.32 | 113.80 |
| 67 | 5 | 4345 | C | N3-C2-O2 | -7.04 | 116.97 | 121.90 |
| 67 | 5 | 301 | G | C2-N3-C4 | -7.04 | 108.38 | 111.90 |
| 67 | 5 | 2320 | G | C2-N3-C4 | -7.04 | 108.38 | 111.90 |
| 73 | 8 | 96 | C | C5-C4-N4 | -7.04 | 115.27 | 120.20 |
| 67 | 5 | 1594 | C | C5-C4-N4 | -7.03 | 115.28 | 120.20 |
| 67 | 5 | 4435 | U | O5'-P-OP1 | -7.03 | 99.38 | 105.70 |
| 67 | 5 | 1456 | C | C5-C4-N4 | -7.02 | 115.28 | 120.20 |
| 13 | FF | 19 | LEU | N-CA-C | -7.02 | 92.04 | 111.00 |
| 67 | 5 | 2302 | C | N1-C2-O2 | 7.02 | 123.11 | 118.90 |
| 67 | 5 | 4394 | A | N1-C6-N6 | 7.02 | 122.81 | 118.60 |
| 67 | 5 | 81 | C | C2-N1-C1' | 7.02 | 126.52 | 118.80 |
| 28 | ii | 232 | PHE | CB-CG-CD1 | 7.02 | 125.71 | 120.80 |
| 67 | 5 | 4981 | G | C8-N9-C1' | -7.01 | 117.89 | 127.00 |
| 67 | 5 | 2659 | A | N1-C6-N6 | 7.01 | 122.81 | 118.60 |
| 67 | 5 | 1662 | C | C6-N1-C1' | -7.01 | 112.39 | 120.80 |
| 67 | 5 | 1847 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 70 | 7 | 95 | C | C2-N1-C1' | 7.00 | 126.50 | 118.80 |
| 67 | 5 | 55 | G | C4-N9-C1' | 7.00 | 135.60 | 126.50 |
| 67 | 5 | 3911 | C | N3-C4-N4 | 7.00 | 122.90 | 118.00 |
| 76 | 9 | 1219 | C | C6-N1-C1' | -7.00 | 112.40 | 120.80 |
| 67 | 5 | 4193 | C | C6-N1-C1' | -6.99 | 112.42 | 120.80 |
| 67 | 5 | 1238 | A | N1-C6-N6 | -6.99 | 114.41 | 118.60 |
| 67 | 5 | 1879 | C | N1-C2-O2 | 6.99 | 123.09 | 118.90 |
| 67 | 5 | 1981 | G | N3-C4-N9 | -6.98 | 121.81 | 126.00 |
| 67 | 5 | 4485 | C | C2-N1-C1' | 6.98 | 126.48 | 118.80 |
| 67 | 5 | 1626 | G | C2-N3-C4 | -6.98 | 108.41 | 111.90 |
| 67 | 5 | 1237 | C | C5-C4-N4 | -6.97 | 115.32 | 120.20 |
| 67 | 5 | 2393 | C | C6-N1-C1' | -6.97 | 112.43 | 120.80 |
| 67 | 5 | 4669 | A | C6-N1-C2 | -6.97 | 114.42 | 118.60 |
| 67 | 5 | 2509 | C | C5-C4-N4 | -6.97 | 115.32 | 120.20 |
| 67 | 5 | 1271 | G | C8-N9-C4 | -6.96 | 103.61 | 106.40 |
| 67 | 5 | 4180 | G | C4-N9-C1' | 6.96 | 135.55 | 126.50 |
| 76 | 9 | 1648 | G | O4'-C1'-N9 | 6.96 | 113.77 | 108.20 |
| 67 | 5 | 238 | C | C6-N1-C2 | -6.96 | 117.52 | 120.30 |
| 67 | 5 | 2393 | C | N1-C2-O2 | 6.96 | 123.07 | 118.90 |
| 67 | 5 | 51 | A | C5-C6-N6 | -6.95 | 118.14 | 123.70 |
| 76 | 9 | 319 | C | O4'-C1'-N1 | 6.95 | 113.76 | 108.20 |
| 76 | 9 | 1191 | C | N3-C4-C5 | 6.95 | 124.68 | 121.90 |
| 67 | 5 | 1064 | G | C4-N9-C1' | 6.95 | 135.53 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 66 | A | O4'-C1'-N9 | 6.95 | 113.76 | 108.20 |
| 67 | 5 | 2836 | A | C2-N3-C4 | -6.95 | 107.13 | 110.60 |
| 76 | 9 | 689 | U | O4'-C1'-N1 | -6.95 | 102.64 | 108.20 |
| 67 | 5 | 1985 | G | C4-N9-C1' | 6.94 | 135.53 | 126.50 |
| 76 | 9 | 876 | C | C2-N1-C1' | 6.94 | 126.43 | 118.80 |
| 67 | 5 | 363 | A | N1-C6-N6 | -6.94 | 114.44 | 118.60 |
| 67 | 5 | 1529 | G | C4-N9-C1' | 6.93 | 135.51 | 126.50 |
| 67 | 5 | 2860 | C | C5-C4-N4 | -6.93 | 115.34 | 120.20 |
| 67 | 5 | 1931 | C | C6-N1-C1' | -6.93 | 112.49 | 120.80 |
| 67 | 5 | 5069 | U | O4'-C1'-N1 | 6.93 | 113.74 | 108.20 |
| 67 | 5 | 1077 | C | N3-C2-O2 | -6.92 | 117.05 | 121.90 |
| 67 | 5 | 1890 | G | C4-C5-N7 | 6.92 | 113.57 | 110.80 |
| 67 | 5 | 2847 | G | O4'-C1'-N9 | 6.92 | 113.74 | 108.20 |
| 73 | 8 | 41 | A | O4'-C1'-N9 | 6.92 | 113.74 | 108.20 |
| 67 | 5 | 302 | C | N3-C2-O2 | -6.92 | 117.05 | 121.90 |
| 67 | 5 | 4215 | C | C6-N1-C2 | 6.92 | 123.07 | 120.30 |
| 73 | 8 | 103 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 67 | 5 | 2693 | G | C8-N9-C1' | -6.92 | 118.01 | 127.00 |
| 67 | 5 | 4179 | G | C8-N9-C1' | -6.92 | 118.01 | 127.00 |
| 67 | 5 | 3650 | C | C6-N1-C1' | -6.91 | 112.50 | 120.80 |
| 67 | 5 | 3774 | A | O4'-C1'-N9 | -6.91 | 102.67 | 108.20 |
| 67 | 5 | 4868 | G | C4-N9-C1' | 6.91 | 135.49 | 126.50 |
| 67 | 5 | 2367 | A | N1-C6-N6 | -6.91 | 114.45 | 118.60 |
| 67 | 5 | 2621 | A | C5-C6-N1 | 6.90 | 121.15 | 117.70 |
| 67 | 5 | 3633 | C | C2-N1-C1' | 6.90 | 126.39 | 118.80 |
| 67 | 5 | 3909 | C | C2-N3-C4 | -6.90 | 116.45 | 119.90 |
| 76 | 9 | 1450 | G | N3-C4-C5 | 6.90 | 132.05 | 128.60 |
| 67 | 5 | 4382 | G | C8-N9-C4 | -6.90 | 103.64 | 106.40 |
| 67 | 5 | 41 | C | N3-C2-O2 | -6.89 | 117.08 | 121.90 |
| 73 | 8 | 26 | C | C2-N1-C1' | 6.89 | 126.38 | 118.80 |
| 76 | 9 | 1460 | C | C6-N1-C2 | -6.89 | 117.55 | 120.30 |
| 70 | 7 | 97 | G | N3-C4-C5 | 6.89 | 132.04 | 128.60 |
| 67 | 5 | 1327 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 67 | 5 | 1847 | C | C6-N1-C1' | -6.88 | 112.55 | 120.80 |
| 67 | 5 | 4705 | A | C5-C6-N1 | 6.87 | 121.14 | 117.70 |
| 67 | 5 | 2878 | G | C6-C5-N7 | -6.87 | 126.28 | 130.40 |
| 67 | 5 | 4375 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 73 | 8 | 26 | C | N1-C2-O2 | 6.87 | 123.02 | 118.90 |
| 67 | 5 | 163 | A | C5-C6-N6 | -6.86 | 118.21 | 123.70 |
| 67 | 5 | 1191 | C | N1-C2-N3 | 6.86 | 124.00 | 119.20 |
| 67 | 5 | 1237 | C | O4'-C1'-N1 | 6.86 | 113.69 | 108.20 |
| 67 | 5 | 70 | A | O4'-C1'-N9 | 6.85 | 113.68 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4919 | G | N9-C4-C5 | -6.85 | 102.66 | 105.40 |
| 67 | 5 | 1329 | G | C4-N9-C1' | 6.85 | 135.41 | 126.50 |
| 67 | 5 | 173 | C | O4'-C1'-N1 | 6.85 | 113.68 | 108.20 |
| 67 | 5 | 2799 | G | N3-C4-C5 | -6.84 | 125.18 | 128.60 |
| 67 | 5 | 2750 | G | N1-C2-N2 | -6.84 | 110.05 | 116.20 |
| 67 | 5 | 84 | A | N1-C6-N6 | 6.84 | 122.70 | 118.60 |
| 67 | 5 | 4179 | G | C8-N9-C4 | -6.84 | 103.67 | 106.40 |
| 67 | 5 | 4985 | U | C6-N1-C2 | -6.84 | 116.90 | 121.00 |
| 67 | 5 | 2393 | C | C2-N1-C1' | 6.83 | 126.31 | 118.80 |
| 67 | 5 | 4528 | G | N7-C8-N9 | 6.82 | 116.51 | 113.10 |
| 67 | 5 | 4696 | C | C5-C4-N4 | -6.82 | 115.42 | 120.20 |
| 67 | 5 | 2784 | C | C5-C4-N4 | -6.82 | 115.42 | 120.20 |
| 67 | 5 | 2836 | A | N1-C6-N6 | 6.82 | 122.69 | 118.60 |
| 67 | 5 | 3737 | A | C5-C6-N6 | -6.82 | 118.25 | 123.70 |
| 76 | 9 | 1513 | C | C6-N1-C2 | -6.82 | 117.57 | 120.30 |
| 67 | 5 | 2603 | C | C5-C4-N4 | -6.82 | 115.43 | 120.20 |
| 67 | 5 | 1665 | C | N3-C2-O2 | -6.82 | 117.13 | 121.90 |
| 73 | 8 | 79 | G | C8-N9-C1' | -6.82 | 118.14 | 127.00 |
| 76 | 9 | 1055 | A | C5-C6-N6 | -6.82 | 118.25 | 123.70 |
| 67 | 5 | 2856 | C | N3-C4-C5 | 6.81 | 124.62 | 121.90 |
| 67 | 5 | 1541 | C | C6-N1-C1' | -6.81 | 112.63 | 120.80 |
| 76 | 9 | 501 | C | N3-C2-O2 | -6.81 | 117.14 | 121.90 |
| 67 | 5 | 3685 | C | C2-N1-C1' | 6.80 | 126.28 | 118.80 |
| 67 | 5 | 2603 | C | C2-N1-C1' | 6.80 | 126.28 | 118.80 |
| 67 | 5 | 4862 | G | N3-C4-C5 | 6.80 | 132.00 | 128.60 |
| 76 | 9 | 1715 | A | C5-C6-N6 | -6.80 | 118.26 | 123.70 |
| 67 | 5 | 3866 | C | N1-C2-O2 | 6.79 | 122.98 | 118.90 |
| 67 | 5 | 4902 | C | N1-C2-O2 | 6.79 | 122.97 | 118.90 |
| 76 | 9 | 1416 | C | C6-N1-C1' | -6.79 | 112.66 | 120.80 |
| 76 | 9 | 1532 | C | N1-C2-O2 | 6.78 | 122.97 | 118.90 |
| 67 | 5 | 1308 | C | C2-N1-C1' | 6.78 | 126.26 | 118.80 |
| 67 | 5 | 1985 | G | P-O3'-C3' | 6.78 | 127.84 | 119.70 |
| 76 | 9 | 475 | C | C6-N1-C2 | 6.78 | 123.01 | 120.30 |
| 67 | 5 | 2848 | G | C2-N3-C4 | -6.78 | 108.51 | 111.90 |
| 67 | 5 | 4738 | C | C5-C4-N4 | -6.78 | 115.45 | 120.20 |
| 76 | 9 | 1216 | C | C5-C4-N4 | 6.78 | 124.94 | 120.20 |
| 67 | 5 | 1623 | A | C5-C6-N6 | -6.78 | 118.28 | 123.70 |
| 67 | 5 | 1641 | G | N3-C4-C5 | 6.78 | 131.99 | 128.60 |
| 73 | 8 | 103 | A | C8-N9-C4 | -6.77 | 103.09 | 105.80 |
| 67 | 5 | 4671 | C | C6-N1-C1' | -6.77 | 112.67 | 120.80 |
| 67 | 5 | 1580 | C | N3-C4-N4 | 6.77 | 122.74 | 118.00 |
| 76 | 9 | 1318 | G | C8-N9-C1' | -6.77 | 118.20 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2785 | C | C2-N1-C1' | 6.77 | 126.24 | 118.80 |
| 76 | 9 | 480 | G | C4-N9-C1' | 6.76 | 135.29 | 126.50 |
| 67 | 5 | 4945 | G | C4-N9-C1' | 6.76 | 135.28 | 126.50 |
| 67 | 5 | 2039 | G | C4-N9-C1' | 6.75 | 135.28 | 126.50 |
| 67 | 5 | 1237 | C | C6-N1-C1' | -6.75 | 112.70 | 120.80 |
| 76 | 9 | 1219 | C | C6-N1-C2 | -6.75 | 117.60 | 120.30 |
| 67 | 5 | 1624 | G | O4'-C1'-N9 | 6.75 | 113.60 | 108.20 |
| 67 | 5 | 3911 | C | C6-N1-C1' | -6.75 | 112.70 | 120.80 |
| 67 | 5 | 355 | A | C6-C5-N7 | -6.74 | 127.58 | 132.30 |
| 67 | 5 | 1599 | G | N3-C2-N2 | 6.74 | 124.62 | 119.90 |
| 67 | 5 | 351 | C | N3-C2-O2 | -6.74 | 117.19 | 121.90 |
| 67 | 5 | 1926 | C | C2-N1-C1' | 6.74 | 126.21 | 118.80 |
| 67 | 5 | 4392 | G | N1-C6-O6 | -6.74 | 115.86 | 119.90 |
| 76 | 9 | 1318 | G | C4-N9-C1' | 6.73 | 135.25 | 126.50 |
| 67 | 5 | 5004 | C | C6-N1-C1' | -6.73 | 112.73 | 120.80 |
| 67 | 5 | 1529 | G | C8-N9-C1' | -6.72 | 118.26 | 127.00 |
| 67 | 5 | 3879 | G | N3-C4-C5 | 6.71 | 131.96 | 128.60 |
| 73 | 8 | 105 | C | C5-C4-N4 | -6.71 | 115.50 | 120.20 |
| 67 | 5 | 1653 | A | C8-N9-C1' | -6.71 | 115.62 | 127.70 |
| 67 | 5 | 3653 | A | C4-C5-C6 | 6.71 | 120.36 | 117.00 |
| 67 | 5 | 4579 | U | C5-C4-O4 | -6.71 | 121.87 | 125.90 |
| 76 | 9 | 1490 | G | C2-N3-C4 | 6.71 | 115.25 | 111.90 |
| 67 | 5 | 2851 | G | C8-N9-C1' | -6.71 | 118.28 | 127.00 |
| 76 | 9 | 1219 | C | C5-C4-N4 | -6.71 | 115.51 | 120.20 |
| 67 | 5 | 1628 | C | N3-C4-N4 | 6.70 | 122.69 | 118.00 |
| 67 | 5 | 4458 | C | C5-C4-N4 | -6.70 | 115.51 | 120.20 |
| 67 | 5 | 336 | A | C5-C6-N1 | 6.70 | 121.05 | 117.70 |
| 67 | 5 | 355 | A | C4-C5-N7 | 6.70 | 114.05 | 110.70 |
| 67 | 5 | 2789 | A | N1-C6-N6 | 6.70 | 122.62 | 118.60 |
| 76 | 9 | 1663 | A | P-O3'-C3' | 6.69 | 127.73 | 119.70 |
| 67 | 5 | 1674 | C | N3-C4-C5 | 6.69 | 124.58 | 121.90 |
| 67 | 5 | 302 | C | C2-N1-C1' | 6.69 | 126.16 | 118.80 |
| 67 | 5 | 1641 | G | C2-N3-C4 | -6.69 | 108.55 | 111.90 |
| 67 | 5 | 4773 | C | O4'-C1'-N1 | -6.69 | 102.85 | 108.20 |
| 67 | 5 | 1076 | C | C6-N1-C2 | -6.68 | 117.63 | 120.30 |
| 67 | 5 | 3623 | C | C6-N1-C1' | -6.68 | 112.78 | 120.80 |
| 76 | 9 | 1603 | G | N3-C4-N9 | 6.68 | 130.01 | 126.00 |
| 67 | 5 | 1315 | C | N3-C4-C5 | 6.68 | 124.57 | 121.90 |
| 67 | 5 | 2057 | A | N1-C6-N6 | -6.68 | 114.59 | 118.60 |
| 67 | 5 | 4886 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 67 | 5 | 3646 | A | C5-C6-N6 | -6.67 | 118.37 | 123.70 |
| 67 | 5 | 1898 | C | N3-C4-C5 | 6.67 | 124.57 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 3760 | A | N1-C6-N6 | -6.66 | 114.60 | 118.60 |
| 76 | 9 | 1824 | A | C5'-C4'-O4' | 6.66 | 117.09 | 109.10 |
| 67 | 5 | 1794 | A | C5-N7-C8 | -6.66 | 100.57 | 103.90 |
| 67 | 5 | 1733 | G | N1-C2-N2 | -6.66 | 110.21 | 116.20 |
| 67 | 5 | 741 | C | C6-N1-C2 | -6.65 | 117.64 | 120.30 |
| 67 | 5 | 4278 | C | C5-C4-N4 | -6.65 | 115.54 | 120.20 |
| 17 | BB | 86 | LEU | CA-CB-CG | 6.65 | 130.59 | 115.30 |
| 76 | 9 | 465 | A | N1-C6-N6 | 6.65 | 122.59 | 118.60 |
| 76 | 9 | 1760 | G | N3-C4-N9 | -6.65 | 122.01 | 126.00 |
| 67 | 5 | 323 | C | N1-C2-O2 | 6.64 | 122.88 | 118.90 |
| 67 | 5 | 2846 | G | N3-C4-C5 | -6.64 | 125.28 | 128.60 |
| 67 | 5 | 352 | G | C8-N9-C1' | -6.64 | 118.37 | 127.00 |
| 67 | 5 | 2465 | C | N3-C2-O2 | -6.64 | 117.25 | 121.90 |
| 67 | 5 | 4701 | A | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 76 | 9 | 810 | A | N9-C1'-C2' | -6.64 | 104.70 | 112.00 |
| 76 | 9 | 1389 | C | C6-N1-C2 | -6.63 | 117.65 | 120.30 |
| 67 | 5 | 1885 | G | C8-N9-C1' | -6.63 | 118.38 | 127.00 |
| 67 | 5 | 2758 | G | C8-N9-C1' | -6.63 | 118.38 | 127.00 |
| 67 | 5 | 4705 | A | C6-N1-C2 | -6.63 | 114.62 | 118.60 |
| 2 | C | 238 | LEU | CA-CB-CG | 6.62 | 130.54 | 115.30 |
| 67 | 5 | 2261 | G | N3-C4-C5 | 6.62 | 131.91 | 128.60 |
| 67 | 5 | 4516 | G | N3-C4-N9 | -6.62 | 122.03 | 126.00 |
| 67 | 5 | 2458 | C | C2-N1-C1' | 6.62 | 126.08 | 118.80 |
| 67 | 5 | 72 | C | N3-C4-C5 | 6.62 | 124.55 | 121.90 |
| 67 | 5 | 1883 | G | C2-N3-C4 | -6.62 | 108.59 | 111.90 |
| 67 | 5 | 4434 | C | C2-N1-C1' | 6.62 | 126.08 | 118.80 |
| 76 | 9 | 1539 | U | O4'-C1'-N1 | 6.62 | 113.49 | 108.20 |
| 67 | 5 | 2299 | G | N3-C4-C5 | -6.62 | 125.29 | 128.60 |
| 67 | 5 | 3867 | A | N1-C6-N6 | 6.61 | 122.57 | 118.60 |
| 76 | 9 | 123 | G | C4-N9-C1' | 6.61 | 135.10 | 126.50 |
| 67 | 5 | 361 | C | O4'-C1'-N1 | 6.61 | 113.49 | 108.20 |
| 67 | 5 | 3749 | C | C6-N1-C1' | -6.61 | 112.87 | 120.80 |
| 67 | 5 | 2838 | G | C8-N9-C4 | -6.61 | 103.76 | 106.40 |
| 84 | cc | 58 | LEU | CA-CB-CG | 6.60 | 130.48 | 115.30 |
| 67 | 5 | 2851 | G | C4-N9-C1' | 6.60 | 135.08 | 126.50 |
| 76 | 9 | 1501 | C | N1-C2-O2 | 6.60 | 122.86 | 118.90 |
| 67 | 5 | 1584 | G | C2-N3-C4 | -6.60 | 108.60 | 111.90 |
| 67 | 5 | 2277 | C | C2-N1-C1' | 6.59 | 126.05 | 118.80 |
| 67 | 5 | 2078 | C | C5-C4-N4 | -6.59 | 115.59 | 120.20 |
| 67 | 5 | 2850 | A | C5-C6-N1 | 6.59 | 120.99 | 117.70 |
| 67 | 5 | 2694 | G | O4'-C1'-N9 | -6.59 | 102.93 | 108.20 |
| 67 | 5 | 84 | A | C5-C6-N6 | -6.58 | 118.43 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1610 | C | C5-C4-N4 | -6.58 | 115.59 | 120.20 |
| 73 | 8 | 26 | C | N3-C4-C5 | 6.58 | 124.53 | 121.90 |
| 67 | 5 | 1331 | C | C5-C4-N4 | -6.58 | 115.60 | 120.20 |
| 67 | 5 | 1864 | G | N3-C4-N9 | 6.57 | 129.94 | 126.00 |
| 76 | 9 | 501 | C | N1-C2-O2 | 6.57 | 122.84 | 118.90 |
| 67 | 5 | 4392 | G | C8-N9-C4 | -6.57 | 103.77 | 106.40 |
| 67 | 5 | 1543 | G | N1-C2-N2 | -6.57 | 110.29 | 116.20 |
| 67 | 5 | 4189 | U | C5-C4-O4 | -6.57 | 121.96 | 125.90 |
| 67 | 5 | 4529 | G | C4-N9-C1' | 6.57 | 135.04 | 126.50 |
| 67 | 5 | 3910 | C | C6-N1-C1' | -6.57 | 112.92 | 120.80 |
| 67 | 5 | 4667 | C | N3-C2-O2 | -6.57 | 117.31 | 121.90 |
| 67 | 5 | 81 | C | C5-C4-N4 | -6.56 | 115.61 | 120.20 |
| 67 | 5 | 1682 | A | N1-C2-N3 | 6.56 | 132.58 | 129.30 |
| 67 | 5 | 3633 | C | N1-C2-O2 | 6.56 | 122.83 | 118.90 |
| 67 | 5 | 54 | G | C8-N9-C1' | -6.55 | 118.48 | 127.00 |
| 67 | 5 | 4180 | G | C8-N9-C1' | -6.55 | 118.48 | 127.00 |
| 67 | 5 | 4256 | A | N1-C6-N6 | 6.55 | 122.53 | 118.60 |
| 67 | 5 | 4510 | A | N1-C6-N6 | 6.55 | 122.53 | 118.60 |
| 67 | 5 | 2075 | G | C8-N9-C1' | -6.55 | 118.48 | 127.00 |
| 67 | 5 | 2629 | C | N1-C2-O2 | 6.54 | 122.83 | 118.90 |
| 76 | 9 | 1637 | A | O4'-C1'-N9 | -6.54 | 102.97 | 108.20 |
| 67 | 5 | 1520 | C | C2-N1-C1' | 6.54 | 125.99 | 118.80 |
| 67 | 5 | 1573 | G | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 67 | 5 | 2834 | C | O4'-C1'-N1 | -6.54 | 102.97 | 108.20 |
| 67 | 5 | 2671 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 67 | 5 | 418 | A | C6-N1-C2 | -6.53 | 114.68 | 118.60 |
| 67 | 5 | 352 | G | C4-N9-C1' | 6.53 | 134.99 | 126.50 |
| 67 | 5 | 1237 | C | C2-N1-C1' | 6.53 | 125.98 | 118.80 |
| 67 | 5 | 89 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 67 | 5 | 2290 | C | O4'-C1'-N1 | 6.53 | 113.42 | 108.20 |
| 67 | 5 | 4715 | C | N1-C2-O2 | 6.53 | 122.82 | 118.90 |
| 76 | 9 | 1191 | C | C5-C4-N4 | -6.53 | 115.63 | 120.20 |
| 67 | 5 | 1926 | C | N1-C2-O2 | 6.53 | 122.81 | 118.90 |
| 67 | 5 | 2074 | C | C5-C4-N4 | -6.53 | 115.63 | 120.20 |
| 67 | 5 | 2802 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 76 | 9 | 1526 | G | N3-C2-N2 | -6.52 | 115.34 | 119.90 |
| 67 | 5 | 2835 | A | C8-N9-C4 | -6.52 | 103.19 | 105.80 |
| 76 | 9 | 1181 | A | N1-C6-N6 | 6.52 | 122.51 | 118.60 |
| 67 | 5 | 1670 | G | N1-C2-N2 | -6.51 | 110.34 | 116.20 |
| 76 | 9 | 168 | C | C2-N1-C1' | 6.51 | 125.97 | 118.80 |
| 35 | KK | 70 | TYR | CA-CB-CG | 6.51 | 125.77 | 113.40 |
| 67 | 5 | 2834 | C | C6-N1-C1' | -6.51 | 112.99 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1465 | G | C6-C5-N7 | -6.51 | 126.50 | 130.40 |
| 67 | 5 | 1306 | C | C5-C4-N4 | -6.51 | 115.64 | 120.20 |
| 67 | 5 | 3882 | C | O4'-C1'-N1 | 6.50 | 113.40 | 108.20 |
| 67 | 5 | 3872 | A | C6-N1-C2 | -6.50 | 114.70 | 118.60 |
| 67 | 5 | 4654 | C | C6-N1-C1' | -6.50 | 113.00 | 120.80 |
| 67 | 5 | 4981 | G | N3-C2-N2 | 6.50 | 124.45 | 119.90 |
| 67 | 5 | 958 | G | C2-N3-C4 | -6.50 | 108.65 | 111.90 |
| 67 | 5 | 2320 | G | N1-C2-N2 | -6.50 | 110.35 | 116.20 |
| 67 | 5 | 4345 | C | N1-C2-O2 | 6.50 | 122.80 | 118.90 |
| 67 | 5 | 1623 | A | C6-C5-N7 | -6.50 | 127.75 | 132.30 |
| 67 | 5 | 4533 | A | C6-C5-N7 | -6.50 | 127.75 | 132.30 |
| 67 | 5 | 66 | A | N1-C6-N6 | -6.50 | 114.70 | 118.60 |
| 67 | 5 | 1305 | C | C2-N1-C1' | 6.49 | 125.94 | 118.80 |
| 67 | 5 | 2012 | A | O4'-C1'-N9 | 6.49 | 113.39 | 108.20 |
| 76 | 9 | 974 | C | C6-N1-C2 | -6.49 | 117.70 | 120.30 |
| 67 | 5 | 3782 | C | C5-C4-N4 | -6.49 | 115.66 | 120.20 |
| 67 | 5 | 4981 | G | C4-N9-C1' | 6.49 | 134.94 | 126.50 |
| 67 | 5 | 1655 | C | C2-N1-C1' | 6.48 | 125.93 | 118.80 |
| 76 | 9 | 1532 | C | C6-N1-C1' | -6.48 | 113.02 | 120.80 |
| 67 | 5 | 360 | A | C5-N7-C8 | -6.48 | 100.66 | 103.90 |
| 76 | 9 | 1834 | A | N1-C6-N6 | 6.48 | 122.49 | 118.60 |
| 67 | 5 | 98 | A | N1-C6-N6 | -6.48 | 114.71 | 118.60 |
| 67 | 5 | 1373 | A | N1-C6-N6 | 6.47 | 122.48 | 118.60 |
| 67 | 5 | 1623 | A | C5-N7-C8 | -6.47 | 100.66 | 103.90 |
| 67 | 5 | 11 | G | C8-N9-C1' | -6.47 | 118.59 | 127.00 |
| 67 | 5 | 1306 | C | N1-C2-O2 | 6.47 | 122.78 | 118.90 |
| 67 | 5 | 1643 | A | C6-N1-C2 | -6.47 | 114.72 | 118.60 |
| 67 | 5 | 314 | G | C8-N9-C4 | -6.47 | 103.81 | 106.40 |
| 67 | 5 | 1853 | G | C2-N3-C4 | -6.46 | 108.67 | 111.90 |
| 67 | 5 | 4680 | G | N1-C2-N2 | -6.46 | 110.38 | 116.20 |
| 67 | 5 | 2850 | A | C8-N9-C4 | -6.46 | 103.22 | 105.80 |
| 67 | 5 | 2743 | A | C5-C6-N1 | 6.46 | 120.93 | 117.70 |
| 61 | TT | 66 | LEU | CA-CB-CG | 6.46 | 130.15 | 115.30 |
| 67 | 5 | 4717 | A | C5-C6-N1 | 6.46 | 120.93 | 117.70 |
| 67 | 5 | 2335 | C | C2-N1-C1' | 6.45 | 125.90 | 118.80 |
| 76 | 9 | 1230 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 76 | 9 | 1452 | A | O5'-P-OP1 | -6.45 | 99.89 | 105.70 |
| 67 | 5 | 30 | C | C2-N1-C1' | 6.45 | 125.89 | 118.80 |
| 67 | 5 | 2533 | C | C2-N1-C1' | 6.45 | 125.89 | 118.80 |
| 63 | UU | 73 | GLY | N-CA-C | -6.45 | 96.99 | 113.10 |
| 67 | 5 | 1342 | A | C8-N9-C4 | -6.44 | 103.22 | 105.80 |
| 67 | 5 | 1427 | A | N9-C4-C5 | -6.44 | 103.22 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 3903 | A | C5-C6-N6 | -6.44 | 118.55 | 123.70 |
| 67 | 5 | 4746 | C | N3-C4-N4 | 6.44 | 122.51 | 118.00 |
| 67 | 5 | 3898 | G | C2-N3-C4 | -6.44 | 108.68 | 111.90 |
| 70 | 7 | 57 | C | C2-N1-C1' | 6.44 | 125.88 | 118.80 |
| 67 | 5 | 1836 | G | N1-C2-N2 | -6.43 | 110.41 | 116.20 |
| 57 | S | 84 | TYR | CB-CG-CD2 | 6.43 | 124.86 | 121.00 |
| 67 | 5 | 3923 | A | C6-N1-C2 | -6.43 | 114.74 | 118.60 |
| 67 | 5 | 4529 | G | C8-N9-C1' | -6.43 | 118.64 | 127.00 |
| 67 | 5 | 4980 | C | N3-C4-N4 | 6.43 | 122.50 | 118.00 |
| 76 | 9 | 563 | G | C4-N9-C1' | 6.43 | 134.86 | 126.50 |
| 76 | 9 | 1658 | G | N9-C4-C5 | -6.43 | 102.83 | 105.40 |
| 67 | 5 | 2320 | G | C8-N9-C1' | -6.42 | 118.65 | 127.00 |
| 84 | cc | 11 | LEU | CB-CG-CD2 | -6.42 | 100.08 | 111.00 |
| 76 | 9 | 84 | A | C4-N9-C1' | 6.42 | 137.86 | 126.30 |
| 67 | 5 | 2577 | C | N1-C2-O2 | 6.42 | 122.75 | 118.90 |
| 67 | 5 | 4924 | C | N1-C2-O2 | 6.42 | 122.75 | 118.90 |
| 73 | 8 | 72 | A | N1-C6-N6 | 6.42 | 122.45 | 118.60 |
| 73 | 8 | 79 | G | O4'-C1'-N9 | -6.42 | 103.06 | 108.20 |
| 67 | 5 | 360 | A | C5-C6-N1 | 6.42 | 120.91 | 117.70 |
| 67 | 5 | 2856 | C | C5-C4-N4 | -6.42 | 115.71 | 120.20 |
| 76 | 9 | 1226 | G | C8-N9-C4 | -6.42 | 103.83 | 106.40 |
| 67 | 5 | 40 | G | N3-C4-C5 | 6.41 | 131.81 | 128.60 |
| 67 | 5 | 4169 | G | C2-N3-C4 | -6.41 | 108.69 | 111.90 |
| 84 | cc | 25 | GLY | N-CA-C | -6.41 | 97.08 | 113.10 |
| 67 | 5 | 387 | G | N3-C4-N9 | 6.41 | 129.84 | 126.00 |
| 67 | 5 | 1298 | C | N1-C2-O2 | 6.41 | 122.74 | 118.90 |
| 67 | 5 | 1682 | A | C5-C6-N6 | -6.40 | 118.58 | 123.70 |
| 67 | 5 | 2540 | C | C2-N1-C1' | 6.40 | 125.84 | 118.80 |
| 67 | 5 | 3771 | C | C6-N1-C2 | -6.40 | 117.74 | 120.30 |
| 67 | 5 | 2841 | G | C8-N9-C4 | -6.40 | 103.84 | 106.40 |
| 67 | 5 | 3683 | C | N3-C4-C5 | 6.40 | 124.46 | 121.90 |
| 67 | 5 | 4456 | C | N1-C2-O2 | 6.40 | 122.74 | 118.90 |
| 67 | 5 | 666 | G | N3-C2-N2 | -6.40 | 115.42 | 119.90 |
| 67 | 5 | 2785 | C | N3-C4-C5 | 6.40 | 124.46 | 121.90 |
| 76 | 9 | 1849 | G | C8-N9-C1' | -6.40 | 118.68 | 127.00 |
| 67 | 5 | 39 | A | C5-C6-N6 | -6.39 | 118.58 | 123.70 |
| 67 | 5 | 112 | C | C6-N1-C1' | -6.39 | 113.13 | 120.80 |
| 67 | 5 | 63 | G | C8-N9-C1' | -6.39 | 118.69 | 127.00 |
| 67 | 5 | 1924 | C | C2-N1-C1' | 6.39 | 125.83 | 118.80 |
| 76 | 9 | 1219 | C | N3-C4-N4 | 6.39 | 122.47 | 118.00 |
| 67 | 5 | 2057 | A | C5-C6-N1 | 6.39 | 120.89 | 117.70 |
| 67 | 5 | 4305 | G | C6-C5-N7 | -6.38 | 126.57 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4667 | C | N1-C2-O2 | 6.38 | 122.73 | 118.90 |
| 76 | 9 | 995 | G | N3-C2-N2 | 6.38 | 124.36 | 119.90 |
| 67 | 5 | 1662 | C | N3-C2-O2 | -6.38 | 117.44 | 121.90 |
| 67 | 5 | 2349 | A | C5-C6-N1 | 6.38 | 120.89 | 117.70 |
| 67 | 5 | 4533 | A | C4-C5-N7 | 6.38 | 113.89 | 110.70 |
| 67 | 5 | 3911 | C | C5-C6-N1 | 6.38 | 124.19 | 121.00 |
| 67 | 5 | 1739 | G | C4-N9-C1' | 6.37 | 134.78 | 126.50 |
| 67 | 5 | 4389 | C | C2-N1-C1' | 6.37 | 125.81 | 118.80 |
| 67 | 5 | 65 | A | O4'-C1'-N9 | 6.37 | 113.30 | 108.20 |
| 67 | 5 | 1520 | C | C6-N1-C1' | -6.37 | 113.16 | 120.80 |
| 67 | 5 | 4688 | C | C2-N1-C1' | 6.37 | 125.80 | 118.80 |
| 67 | 5 | 3917 | A | C5-C6-N1 | 6.36 | 120.88 | 117.70 |
| 67 | 5 | 4195 | G | N1-C2-N2 | -6.36 | 110.47 | 116.20 |
| 67 | 5 | 4527 | G | C8-N9-C1' | -6.36 | 118.73 | 127.00 |
| 67 | 5 | 1733 | G | N3-C2-N2 | 6.36 | 124.35 | 119.90 |
| 67 | 5 | 1864 | G | C4-N9-C1' | 6.36 | 134.76 | 126.50 |
| 67 | 5 | 2863 | G | C2-N3-C4 | -6.36 | 108.72 | 111.90 |
| 67 | 5 | 4549 | G | N1-C2-N2 | -6.35 | 110.48 | 116.20 |
| 73 | 8 | 41 | A | N9-C4-C5 | 6.35 | 108.34 | 105.80 |
| 76 | 9 | 1638 | G | C4-N9-C1' | -6.35 | 118.24 | 126.50 |
| 67 | 5 | 2638 | G | N3-C4-C5 | 6.34 | 131.77 | 128.60 |
| 67 | 5 | 4726 | G | N3-C4-N9 | -6.34 | 122.19 | 126.00 |
| 76 | 9 | 1305 | C | N1-C2-O2 | 6.34 | 122.71 | 118.90 |
| 57 | S | 84 | TYR | CB-CG-CD1 | -6.34 | 117.19 | 121.00 |
| 67 | 5 | 1944 | A | C5-C6-N6 | -6.34 | 118.63 | 123.70 |
| 67 | 5 | 4088 | C | N1-C2-O2 | 6.34 | 122.70 | 118.90 |
| 76 | 9 | 987 | A | O4'-C1'-N9 | -6.34 | 103.13 | 108.20 |
| 67 | 5 | 108 | A | N1-C6-N6 | 6.34 | 122.40 | 118.60 |
| 76 | 9 | 1294 | G | N3-C4-N9 | 6.34 | 129.80 | 126.00 |
| 67 | 5 | 3622 | C | C5-C4-N4 | -6.33 | 115.77 | 120.20 |
| 76 | 9 | 1490 | G | C4-N9-C1' | 6.33 | 134.73 | 126.50 |
| 67 | 5 | 4165 | C | C6-N1-C2 | -6.33 | 117.77 | 120.30 |
| 67 | 5 | 4862 | G | N3-C4-N9 | -6.33 | 122.20 | 126.00 |
| 67 | 5 | 666 | G | N3-C4-N9 | -6.33 | 122.20 | 126.00 |
| 76 | 9 | 1095 | U | C5-C6-N1 | 6.33 | 125.86 | 122.70 |
| 67 | 5 | 4278 | C | C2-N1-C1' | 6.33 | 125.76 | 118.80 |
| 76 | 9 | 42 | A | O4'-C1'-N9 | 6.33 | 113.26 | 108.20 |
| 67 | 5 | 386 | A | C5-C6-N6 | -6.32 | 118.64 | 123.70 |
| 67 | 5 | 1331 | C | C2-N1-C1' | 6.32 | 125.76 | 118.80 |
| 67 | 5 | 2834 | C | C2-N1-C1' | 6.32 | 125.75 | 118.80 |
| 76 | 9 | 52 | G | C2-N3-C4 | -6.32 | 108.74 | 111.90 |
| 67 | 5 | 2519 | U | O4'-C1'-N1 | 6.32 | 113.26 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2354 | G | N1-C2-N2 | -6.32 | 110.51 | 116.20 |
| 67 | 5 | 3903 | A | C4-C5-N7 | 6.32 | 113.86 | 110.70 |
| 76 | 9 | 1717 | C | N1-C2-O2 | 6.32 | 122.69 | 118.90 |
| 67 | 5 | 1535 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 67 | 5 | 1887 | G | C8-N9-C1' | -6.32 | 118.79 | 127.00 |
| 67 | 5 | 4680 | G | C4-N9-C1' | 6.32 | 134.71 | 126.50 |
| 67 | 5 | 4881 | U | N1-C1'-C2' | -6.32 | 105.05 | 112.00 |
| 67 | 5 | 5016 | A | C4-C5-N7 | 6.31 | 113.86 | 110.70 |
| 67 | 5 | 4124 | G | C8-N9-C1' | -6.31 | 118.79 | 127.00 |
| 67 | 5 | 1629 | G | C8-N9-C1' | -6.31 | 118.80 | 127.00 |
| 73 | 8 | 141 | C | N3-C2-O2 | -6.31 | 117.48 | 121.90 |
| 67 | 5 | 2784 | C | N3-C4-C5 | 6.31 | 124.42 | 121.90 |
| 67 | 5 | 1589 | C | C2-N1-C1' | 6.31 | 125.74 | 118.80 |
| 73 | 8 | 6 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 67 | 5 | 3882 | C | C2-N1-C1' | 6.30 | 125.73 | 118.80 |
| 67 | 5 | 23 | C | N1-C1'-C2' | -6.30 | 105.07 | 112.00 |
| 28 | ii | 226 | LEU | CB-CG-CD1 | 6.30 | 121.71 | 111.00 |
| 67 | 5 | 353 | A | C8-N9-C1' | -6.30 | 116.36 | 127.70 |
| 67 | 5 | 2659 | A | C5-C6-N6 | -6.30 | 118.66 | 123.70 |
| 67 | 5 | 1580 | C | N1-C2-O2 | 6.30 | 122.68 | 118.90 |
| 67 | 5 | 2406 | G | C8-N9-C1' | -6.30 | 118.81 | 127.00 |
| 67 | 5 | 163 | A | C5-C6-N1 | 6.29 | 120.85 | 117.70 |
| 67 | 5 | 1924 | C | N3-C2-O2 | -6.29 | 117.50 | 121.90 |
| 67 | 5 | 1574 | G | N1-C2-N2 | -6.29 | 110.54 | 116.20 |
| 67 | 5 | 1640 | C | N3-C4-C5 | 6.29 | 124.42 | 121.90 |
| 67 | 5 | 1235 | G | C5-C6-O6 | 6.29 | 132.37 | 128.60 |
| 67 | 5 | 1529 | G | C8-N9-C4 | -6.28 | 103.89 | 106.40 |
| 76 | 9 | 1526 | G | N1-C2-N2 | 6.28 | 121.85 | 116.20 |
| 67 | 5 | 4166 | G | N1-C2-N2 | -6.28 | 110.55 | 116.20 |
| 67 | 5 | 1967 | A | C5-C6-N6 | -6.28 | 118.68 | 123.70 |
| 67 | 5 | 3893 | C | N1-C2-O2 | 6.27 | 122.66 | 118.90 |
| 67 | 5 | 1373 | A | C6-C5-N7 | -6.27 | 127.91 | 132.30 |
| 67 | 5 | 1373 | A | N9-C4-C5 | -6.27 | 103.29 | 105.80 |
| 67 | 5 | 1651 | G | N3-C2-N2 | 6.27 | 124.29 | 119.90 |
| 67 | 5 | 2638 | G | N3-C4-N9 | -6.27 | 122.24 | 126.00 |
| 67 | 5 | 3598 | C | O4'-C1'-N1 | 6.27 | 113.21 | 108.20 |
| 67 | 5 | 2025 | A | N9-C4-C5 | -6.27 | 103.29 | 105.80 |
| 67 | 5 | 4375 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 41 | MM | 33 | ARG | C-N-CA | 6.26 | 135.44 | 122.30 |
| 67 | 5 | 324 | A | C5-C6-N1 | 6.26 | 120.83 | 117.70 |
| 67 | 5 | 4447 | C | C5-C4-N4 | -6.26 | 115.82 | 120.20 |
| 67 | 5 | 494 | C | N3-C4-N4 | -6.25 | 113.62 | 118.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 55 | G | C8-N9-C1' | -6.25 | 118.87 | 127.00 |
| 67 | 5 | 4561 | C | C6-N1-C1' | -6.25 | 113.30 | 120.80 |
| 67 | 5 | 2838 | G | C6-C5-N7 | -6.25 | 126.65 | 130.40 |
| 67 | 5 | 4444 | C | N1-C2-O2 | 6.25 | 122.65 | 118.90 |
| 67 | 5 | 1944 | A | C5-C6-N1 | 6.25 | 120.82 | 117.70 |
| 67 | 5 | 2533 | C | C6-N1-C1' | -6.25 | 113.30 | 120.80 |
| 67 | 5 | 4948 | C | C5-C4-N4 | -6.25 | 115.83 | 120.20 |
| 76 | 9 | 1498 | A | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 67 | 5 | 1739 | G | N3-C4-C5 | -6.24 | 125.48 | 128.60 |
| 76 | 9 | 1148 | A | N1-C6-N6 | 6.24 | 122.34 | 118.60 |
| 67 | 5 | 1812 | C | C6-N1-C2 | -6.24 | 117.81 | 120.30 |
| 67 | 5 | 4451 | G | N1-C2-N2 | -6.24 | 110.59 | 116.20 |
| 67 | 5 | 4561 | C | C2-N1-C1' | 6.24 | 125.66 | 118.80 |
| 67 | 5 | 2041 | A | N1-C6-N6 | -6.23 | 114.86 | 118.60 |
| 67 | 5 | 1623 | A | C4-C5-N7 | 6.23 | 113.81 | 110.70 |
| 67 | 5 | 3897 | G | C2-N3-C4 | -6.23 | 108.78 | 111.90 |
| 83 | CC | 66 | LEU | CA-CB-CG | 6.23 | 129.63 | 115.30 |
| 67 | 5 | 719 | C | N1-C2-O2 | 6.23 | 122.64 | 118.90 |
| 67 | 5 | 1535 | C | C2-N3-C4 | -6.23 | 116.79 | 119.90 |
| 67 | 5 | 1674 | C | C6-N1-C1' | -6.23 | 113.33 | 120.80 |
| 67 | 5 | 4434 | C | C6-N1-C1' | -6.23 | 113.33 | 120.80 |
| 67 | 5 | 1387 | A | C5-C6-N6 | -6.23 | 118.72 | 123.70 |
| 67 | 5 | 4761 | G | N3-C4-C5 | 6.23 | 131.71 | 128.60 |
| 67 | 5 | 4624 | A | C6-N1-C2 | -6.22 | 114.87 | 118.60 |
| 76 | 9 | 1603 | G | O4'-C1'-N9 | 6.22 | 113.17 | 108.20 |
| 28 | ii | 68 | ARG | NE-CZ-NH2 | 6.22 | 123.41 | 120.30 |
| 67 | 5 | 4579 | U | C2-N1-C1' | 6.22 | 125.16 | 117.70 |
| 76 | 9 | 140 | U | C2-N1-C1' | 6.22 | 125.16 | 117.70 |
| 67 | 5 | 2406 | G | C4-N9-C1' | 6.21 | 134.58 | 126.50 |
| 76 | 9 | 1389 | C | C2-N1-C1' | 6.21 | 125.63 | 118.80 |
| 67 | 5 | 83 | C | C6-N1-C2 | 6.21 | 122.78 | 120.30 |
| 76 | 9 | 171 | A | C5-C6-N6 | -6.21 | 118.73 | 123.70 |
| 76 | 9 | 662 | G | O4'-C1'-N9 | -6.21 | 103.23 | 108.20 |
| 76 | 9 | 106 | C | N1-C2-O2 | 6.21 | 122.62 | 118.90 |
| 67 | 5 | 4305 | G | C4-C5-N7 | 6.20 | 113.28 | 110.80 |
| 67 | 5 | 4305 | G | C8-N9-C4 | -6.19 | 103.92 | 106.40 |
| 76 | 9 | 1566 | G | C4-N9-C1' | -6.19 | 118.45 | 126.50 |
| 67 | 5 | 364 | G | C4-C5-N7 | 6.19 | 113.28 | 110.80 |
| 76 | 9 | 1781 | A | N1-C6-N6 | 6.19 | 122.32 | 118.60 |
| 67 | 5 | 1868 | A | N7-C8-N9 | 6.19 | 116.89 | 113.80 |
| 67 | 5 | 2838 | G | N7-C8-N9 | 6.19 | 116.20 | 113.10 |
| 76 | 9 | 1666 | C | C6-N1-C2 | 6.19 | 122.78 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 64 | A | C4-C5-N7 | 6.19 | 113.79 | 110.70 |
| 32 | jj | 426 | LEU | CA-CB-CG | 6.19 | 129.53 | 115.30 |
| 67 | 5 | 2399 | G | N3-C4-C5 | -6.19 | 125.51 | 128.60 |
| 76 | 9 | 621 | C | N1-C2-O2 | 6.19 | 122.61 | 118.90 |
| 67 | 5 | 3869 | C | C5-C4-N4 | -6.19 | 115.87 | 120.20 |
| 67 | 5 | 1803 | G | C8-N9-C1' | -6.18 | 118.96 | 127.00 |
| 67 | 5 | 4528 | G | C4-N9-C1' | 6.18 | 134.54 | 126.50 |
| 67 | 5 | 4696 | C | N3-C4-N4 | 6.18 | 122.33 | 118.00 |
| 76 | 9 | 1438 | A | N1-C6-N6 | 6.18 | 122.31 | 118.60 |
| 67 | 5 | 924 | C | O4'-C1'-N1 | 6.18 | 113.14 | 108.20 |
| 67 | 5 | 2335 | C | C6-N1-C1' | -6.18 | 113.38 | 120.80 |
| 67 | 5 | 3820 | G | C8-N9-C1' | -6.18 | 118.97 | 127.00 |
| 67 | 5 | 4454 | G | N1-C2-N2 | -6.18 | 110.64 | 116.20 |
| 67 | 5 | 1629 | G | C6-C5-N7 | -6.17 | 126.69 | 130.40 |
| 67 | 5 | 2894 | A | C5-C6-N1 | 6.17 | 120.79 | 117.70 |
| 67 | 5 | 4363 | A | C5-C6-N1 | 6.17 | 120.79 | 117.70 |
| 76 | 9 | 621 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 76 | 9 | 1267 | C | O4'-C1'-N1 | 6.17 | 113.14 | 108.20 |
| 67 | 5 | 101 | A | C5-C6-N6 | -6.17 | 118.77 | 123.70 |
| 67 | 5 | 1880 | G | C6-C5-N7 | -6.17 | 126.70 | 130.40 |
| 67 | 5 | 1985 | G | C8-N9-C1' | -6.17 | 118.98 | 127.00 |
| 67 | 5 | 2657 | G | O4'-C1'-N9 | -6.17 | 103.27 | 108.20 |
| 67 | 5 | 299 | C | C2-N1-C1' | 6.16 | 125.58 | 118.80 |
| 67 | 5 | 40 | G | C2-N3-C4 | -6.16 | 108.82 | 111.90 |
| 67 | 5 | 2670 | C | C2-N1-C1' | 6.16 | 125.58 | 118.80 |
| 76 | 9 | 1474 | A | C4-C5-N7 | -6.16 | 107.62 | 110.70 |
| 32 | jj | 292 | PHE | CB-CG-CD2 | -6.16 | 116.49 | 120.80 |
| 67 | 5 | 2639 | U | O4'-C1'-N1 | 6.16 | 113.13 | 108.20 |
| 76 | 9 | 102 | A | O4'-C1'-N9 | 6.16 | 113.13 | 108.20 |
| 76 | 9 | 1860 | A | C5-C6-N1 | 6.16 | 120.78 | 117.70 |
| 76 | 9 | 480 | G | C8-N9-C1' | -6.16 | 119.00 | 127.00 |
| 67 | 5 | 3653 | A | N7-C8-N9 | 6.16 | 116.88 | 113.80 |
| 67 | 5 | 4337 | C | C5-C4-N4 | -6.16 | 115.89 | 120.20 |
| 76 | 9 | 1842 | C | C6-N1-C2 | -6.16 | 117.84 | 120.30 |
| 67 | 5 | 1653 | A | C5-C6-N6 | -6.15 | 118.78 | 123.70 |
| 67 | 5 | 4375 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 67 | 5 | 263 | G | C8-N9-C1' | -6.15 | 119.00 | 127.00 |
| 67 | 5 | 4380 | A | C5-C6-N1 | 6.15 | 120.77 | 117.70 |
| 67 | 5 | 4561 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 76 | 9 | 1806 | A | N1-C6-N6 | 6.15 | 122.29 | 118.60 |
| 67 | 5 | 1759 | G | C8-N9-C4 | -6.15 | 103.94 | 106.40 |
| 67 | 5 | 1342 | A | N7-C8-N9 | 6.14 | 116.87 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2694 | G | C8-N9-C1' | -6.14 | 119.01 | 127.00 |
| 67 | 5 | 3860 | A | C5-C6-N6 | 6.14 | 128.62 | 123.70 |
| 67 | 5 | 3816 | A | O4'-C1'-N9 | 6.14 | 113.11 | 108.20 |
| 67 | 5 | 2878 | G | C8-N9-C1' | -6.14 | 119.02 | 127.00 |
| 67 | 5 | 1854 | G | N1-C2-N2 | -6.14 | 110.68 | 116.20 |
| 67 | 5 | 4331 | G | N3-C2-N2 | 6.14 | 124.20 | 119.90 |
| 67 | 5 | 2443 | G | C4-N9-C1' | 6.13 | 134.47 | 126.50 |
| 67 | 5 | 1690 | C | C2-N1-C1' | 6.13 | 125.54 | 118.80 |
| 67 | 5 | 11 | G | N3-C4-C5 | -6.13 | 125.54 | 128.60 |
| 67 | 5 | 4443 | C | C5-C4-N4 | -6.13 | 115.91 | 120.20 |
| 67 | 5 | 1484 | G | N3-C2-N2 | 6.12 | 124.19 | 119.90 |
| 76 | 9 | 1793 | A | C5-C6-N6 | -6.12 | 118.80 | 123.70 |
| 67 | 5 | 1910 | G | C4-N9-C1' | 6.12 | 134.46 | 126.50 |
| 67 | 5 | 289 | C | C2-N1-C1' | 6.12 | 125.53 | 118.80 |
| 67 | 5 | 4717 | A | C6-N1-C2 | -6.12 | 114.93 | 118.60 |
| 76 | 9 | 123 | G | N3-C4-N9 | 6.12 | 129.67 | 126.00 |
| 67 | 5 | 38 | A | C5-N7-C8 | -6.12 | 100.84 | 103.90 |
| 67 | 5 | 2096 | G | N1-C6-O6 | -6.12 | 116.23 | 119.90 |
| 76 | 9 | 1065 | G | N3-C2-N2 | 6.12 | 124.18 | 119.90 |
| 76 | 9 | 1534 | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 67 | 5 | 3771 | C | C5-C6-N1 | 6.11 | 124.06 | 121.00 |
| 76 | 9 | 84 | A | N1-C6-N6 | 6.11 | 122.27 | 118.60 |
| 76 | 9 | 1294 | G | C4-N9-C1' | 6.11 | 134.45 | 126.50 |
| 70 | 7 | 101 | A | C8-N9-C4 | -6.11 | 103.36 | 105.80 |
| 67 | 5 | 3904 | G | O4'-C1'-N9 | 6.11 | 113.09 | 108.20 |
| 67 | 5 | 4279 | A | N9-C4-C5 | -6.11 | 103.36 | 105.80 |
| 76 | 9 | 1216 | C | C2-N1-C1' | -6.11 | 112.08 | 118.80 |
| 76 | 9 | 674 | C | N3-C4-C5 | 6.11 | 124.34 | 121.90 |
| 67 | 5 | 3687 | A | C5-C6-N6 | -6.11 | 118.82 | 123.70 |
| 67 | 5 | 4661 | G | N1-C2-N3 | 6.11 | 127.56 | 123.90 |
| 67 | 5 | 353 | A | N1-C6-N6 | 6.10 | 122.26 | 118.60 |
| 67 | 5 | 2046 | G | C4-N9-C1' | 6.10 | 134.43 | 126.50 |
| 67 | 5 | 1458 | C | C5-C4-N4 | -6.10 | 115.93 | 120.20 |
| 67 | 5 | 1870 | C | C2-N3-C4 | -6.10 | 116.85 | 119.90 |
| 67 | 5 | 1670 | G | N3-C4-N9 | 6.10 | 129.66 | 126.00 |
| 67 | 5 | 3893 | C | N3-C2-O2 | -6.10 | 117.63 | 121.90 |
| 76 | 9 | 670 | A | C8-N9-C4 | -6.10 | 103.36 | 105.80 |
| 76 | 9 | 995 | G | N1-C2-N2 | -6.10 | 110.71 | 116.20 |
| 67 | 5 | 355 | A | N9-C4-C5 | -6.10 | 103.36 | 105.80 |
| 67 | 5 | 1929 | A | C8-N9-C1' | -6.10 | 116.73 | 127.70 |
| 67 | 5 | 2024 | G | N3-C4-C5 | 6.10 | 131.65 | 128.60 |
| 76 | 9 | 1658 | G | N3-C4-N9 | 6.10 | 129.66 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 3771 | C | C6-N1-C1' | -6.09 | 113.49 | 120.80 |
| 67 | 5 | 4550 | G | N1-C2-N2 | -6.09 | 110.72 | 116.20 |
| 76 | 9 | 1414 | A | N1-C6-N6 | 6.09 | 122.26 | 118.60 |
| 67 | 5 | 1331 | C | C6-N1-C1' | -6.09 | 113.49 | 120.80 |
| 6 | D | 109 | LEU | CB-CG-CD1 | -6.09 | 100.64 | 111.00 |
| 67 | 5 | 356 | G | C8-N9-C1' | -6.09 | 119.08 | 127.00 |
| 67 | 5 | 1734 | G | C2-N3-C4 | -6.09 | 108.85 | 111.90 |
| 72 | Y | 27 | ARG | NE-CZ-NH1 | -6.09 | 117.25 | 120.30 |
| 70 | 7 | 29 | C | N1-C2-O2 | 6.09 | 122.55 | 118.90 |
| 67 | 5 | 1880 | G | N3-C2-N2 | 6.09 | 124.16 | 119.90 |
| 76 | 9 | 1245 | G | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 67 | 5 | 2290 | C | N3-C2-O2 | -6.09 | 117.64 | 121.90 |
| 67 | 5 | 2867 | C | C6-N1-C2 | -6.09 | 117.86 | 120.30 |
| 67 | 5 | 2802 | C | C2-N1-C1' | 6.08 | 125.49 | 118.80 |
| 67 | 5 | 4651 | A | C6-N1-C2 | -6.08 | 114.95 | 118.60 |
| 67 | 5 | 4710 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 67 | 5 | 2746 | A | N1-C6-N6 | 6.08 | 122.25 | 118.60 |
| 67 | 5 | 3719 | A | N1-C6-N6 | 6.08 | 122.25 | 118.60 |
| 67 | 5 | 415 | G | C8-N9-C1' | -6.08 | 119.10 | 127.00 |
| 67 | 5 | 3633 | C | C6-N1-C1' | -6.08 | 113.51 | 120.80 |
| 67 | 5 | 4942 | C | P-O3'-C3' | 6.08 | 126.99 | 119.70 |
| 59 | SS | 137 | LYS | CA-CB-CG | 6.08 | 126.77 | 113.40 |
| 67 | 5 | 355 | A | C5-N7-C8 | -6.08 | 100.86 | 103.90 |
| 67 | 5 | 1836 | G | O4'-C1'-N9 | 6.08 | 113.06 | 108.20 |
| 67 | 5 | 1916 | G | C4-N9-C1' | 6.08 | 134.40 | 126.50 |
| 67 | 5 | 2379 | A | C8-N9-C1' | -6.08 | 116.77 | 127.70 |
| 67 | 5 | 2878 | G | N1-C2-N2 | -6.08 | 110.73 | 116.20 |
| 67 | 5 | 3687 | A | N1-C6-N6 | 6.08 | 122.25 | 118.60 |
| 67 | 5 | 3924 | C | C2-N1-C1' | 6.08 | 125.48 | 118.80 |
| 67 | 5 | 2014 | C | O4'-C1'-N1 | 6.07 | 113.06 | 108.20 |
| 67 | 5 | 4284 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 76 | 9 | 915 | G | C8-N9-C1' | -6.07 | 119.11 | 127.00 |
| 67 | 5 | 1521 | C | N3-C4-N4 | 6.07 | 122.25 | 118.00 |
| 67 | 5 | 2277 | C | C6-N1-C1' | -6.07 | 113.52 | 120.80 |
| 67 | 5 | 1890 | G | C5-N7-C8 | -6.07 | 101.27 | 104.30 |
| 67 | 5 | 4388 | A | N1-C6-N6 | -6.06 | 114.96 | 118.60 |
| 67 | 5 | 2324 | C | C2-N1-C1' | 6.06 | 125.47 | 118.80 |
| 67 | 5 | 3636 | C | N1-C2-O2 | 6.06 | 122.53 | 118.90 |
| 67 | 5 | 1576 | G | C4-N9-C1' | 6.06 | 134.37 | 126.50 |
| 67 | 5 | 4087 | G | N3-C4-C5 | 6.06 | 131.63 | 128.60 |
| 76 | 9 | 1014 | G | C8-N9-C1' | -6.06 | 119.12 | 127.00 |
| 67 | 5 | 105 | A | C4-C5-N7 | 6.06 | 113.73 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2619 | G | N1-C2-N2 | -6.05 | 110.75 | 116.20 |
| 67 | 5 | 1065 | G | C6-C5-N7 | 6.05 | 134.03 | 130.40 |
| 67 | 5 | 1957 | U | C2-N1-C1' | -6.05 | 110.44 | 117.70 |
| 67 | 5 | 2860 | C | C6-N1-C1' | -6.05 | 113.54 | 120.80 |
| 76 | 9 | 1466 | G | N3-C4-N9 | -6.05 | 122.37 | 126.00 |
| 76 | 9 | 1584 | G | C4-N9-C1' | 6.05 | 134.37 | 126.50 |
| 67 | 5 | 3929 | G | C4-N9-C1' | 6.05 | 134.36 | 126.50 |
| 67 | 5 | 1206 | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 67 | 5 | 5016 | A | C6-C5-N7 | -6.05 | 128.07 | 132.30 |
| 76 | 9 | 84 | A | C4-C5-C6 | 6.05 | 120.02 | 117.00 |
| 67 | 5 | 1318 | C | N3-C4-N4 | 6.04 | 122.23 | 118.00 |
| 67 | 5 | 2319 | C | N3-C4-C5 | 6.04 | 124.32 | 121.90 |
| 73 | 8 | 103 | A | N7-C8-N9 | 6.04 | 116.82 | 113.80 |
| 76 | 9 | 909 | G | C5-C6-O6 | -6.04 | 124.97 | 128.60 |
| 67 | 5 | 1869 | G | C8-N9-C1' | -6.04 | 119.15 | 127.00 |
| 67 | 5 | 3845 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 67 | 5 | 3866 | C | N3-C2-O2 | -6.04 | 117.67 | 121.90 |
| 76 | 9 | 84 | A | C8-N9-C1' | -6.04 | 116.83 | 127.70 |
| 76 | 9 | 1055 | A | C6-C5-N7 | -6.04 | 128.07 | 132.30 |
| 76 | 9 | 1265 | A | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 67 | 5 | 2406 | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |
| 67 | 5 | 2511 | A | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 67 | 5 | 1629 | G | C2-N3-C4 | -6.04 | 108.88 | 111.90 |
| 67 | 5 | 4472 | G | C4-N9-C1' | 6.04 | 134.35 | 126.50 |
| 67 | 5 | 4513 | A | C5-C6-N1 | 6.04 | 120.72 | 117.70 |
| 67 | 5 | 1859 | C | N3-C4-N4 | 6.04 | 122.23 | 118.00 |
| 76 | 9 | 1717 | C | C2-N1-C1' | 6.04 | 125.44 | 118.80 |
| 67 | 5 | 3635 | A | C8-N9-C4 | 6.04 | 108.21 | 105.80 |
| 67 | 5 | 3901 | A | C8-N9-C1' | -6.04 | 116.84 | 127.70 |
| 67 | 5 | 4097 | G | C2-N3-C4 | -6.03 | 108.88 | 111.90 |
| 67 | 5 | 968 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 67 | 5 | 2345 | G | N1-C2-N2 | -6.03 | 110.77 | 116.20 |
| 67 | 5 | 294 | G | N1-C2-N2 | -6.03 | 110.77 | 116.20 |
| 67 | 5 | 4681 | A | C8-N9-C4 | 6.03 | 108.21 | 105.80 |
| 67 | 5 | 41 | C | C6-N1-C1' | -6.03 | 113.57 | 120.80 |
| 67 | 5 | 1926 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 67 | 5 | 351 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 67 | 5 | 1989 | G | N1-C2-N2 | -6.03 | 110.78 | 116.20 |
| 67 | 5 | 2393 | C | N3-C4-C5 | 6.02 | 124.31 | 121.90 |
| 67 | 5 | 2799 | G | N1-C2-N3 | 6.02 | 127.51 | 123.90 |
| 67 | 5 | 4661 | G | C2-N3-C4 | -6.02 | 108.89 | 111.90 |
| 67 | 5 | 4945 | G | C6-C5-N7 | -6.02 | 126.79 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 293 | G | C4-N9-C1' | 6.02 | 134.32 | 126.50 |
| 67 | 5 | 1333 | A | C6-N1-C2 | -6.02 | 114.99 | 118.60 |
| 67 | 5 | 4427 | G | C8-N9-C1' | -6.02 | 119.17 | 127.00 |
| 67 | 5 | 1801 | A | C5-C6-N6 | -6.02 | 118.89 | 123.70 |
| 67 | 5 | 48 | G | N1-C2-N2 | -6.01 | 110.79 | 116.20 |
| 67 | 5 | 2448 | G | N1-C2-N2 | -6.01 | 110.79 | 116.20 |
| 67 | 5 | 1663 | C | C2-N1-C1' | 6.01 | 125.41 | 118.80 |
| 67 | 5 | 1729 | A | C5-C6-N1 | 6.01 | 120.70 | 117.70 |
| 67 | 5 | 1794 | A | C8-N9-C1' | -6.01 | 116.88 | 127.70 |
| 67 | 5 | 1916 | G | C8-N9-C1' | -6.01 | 119.19 | 127.00 |
| 67 | 5 | 2613 | C | N3-C4-C5 | 6.01 | 124.30 | 121.90 |
| 76 | 9 | 1257 | G | C8-N9-C1' | 6.01 | 134.81 | 127.00 |
| 4 | DD | 218 | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 67 | 5 | 1065 | G | C4-N9-C1' | -6.01 | 118.69 | 126.50 |
| 67 | 5 | 2622 | G | C4-N9-C1' | 6.00 | 134.31 | 126.50 |
| 67 | 5 | 3650 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 76 | 9 | 1584 | G | C8-N9-C1' | -6.00 | 119.19 | 127.00 |
| 32 | jj | 632 | LEU | CB-CG-CD1 | -6.00 | 100.80 | 111.00 |
| 67 | 5 | 1458 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 67 | 5 | 2659 | A | N9-C4-C5 | -6.00 | 103.40 | 105.80 |
| 67 | 5 | 2860 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 67 | 5 | 418 | A | C8-N9-C1' | -6.00 | 116.90 | 127.70 |
| 67 | 5 | 3774 | A | C4-N9-C1' | 6.00 | 137.10 | 126.30 |
| 67 | 5 | 3774 | A | C4-C5-N7 | 6.00 | 113.70 | 110.70 |
| 76 | 9 | 501 | C | C6-N1-C2 | -6.00 | 117.90 | 120.30 |
| 67 | 5 | 1329 | G | N3-C4-C5 | -6.00 | 125.60 | 128.60 |
| 76 | 9 | 1566 | G | C8-N9-C1' | 5.99 | 134.79 | 127.00 |
| 67 | 5 | 1371 | A | N1-C6-N6 | 5.99 | 122.19 | 118.60 |
| 67 | 5 | 2321 | G | C2-N3-C4 | -5.99 | 108.91 | 111.90 |
| 67 | 5 | 2379 | A | O4'-C1'-N9 | -5.99 | 103.41 | 108.20 |
| 67 | 5 | 3887 | C | N3-C4-C5 | 5.99 | 124.30 | 121.90 |
| 67 | 5 | 2613 | C | C5-C4-N4 | -5.99 | 116.01 | 120.20 |
| 67 | 5 | 3650 | C | N3-C2-O2 | -5.99 | 117.71 | 121.90 |
| 18 | GG | 133 | LEU | CA-CB-CG | 5.99 | 129.06 | 115.30 |
| 67 | 5 | 1653 | A | C4-C5-N7 | 5.98 | 113.69 | 110.70 |
| 67 | 5 | 2640 | G | C8-N9-C1' | -5.98 | 119.22 | 127.00 |
| 67 | 5 | 2848 | G | N1-C6-O6 | 5.98 | 123.49 | 119.90 |
| 67 | 5 | 2040 | A | N1-C6-N6 | 5.98 | 122.19 | 118.60 |
| 67 | 5 | 1655 | C | C6-N1-C1' | -5.98 | 113.62 | 120.80 |
| 76 | 9 | 1798 | C | N1-C2-O2 | 5.98 | 122.49 | 118.90 |
| 67 | 5 | 323 | C | N3-C2-O2 | -5.98 | 117.71 | 121.90 |
| 67 | 5 | 1323 | A | C4-C5-N7 | 5.98 | 113.69 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4936 | G | N3-C4-C5 | 5.98 | 131.59 | 128.60 |
| 67 | 5 | 1681 | G | N1-C2-N2 | -5.98 | 110.82 | 116.20 |
| 76 | 9 | 171 | A | N1-C6-N6 | 5.98 | 122.19 | 118.60 |
| 67 | 5 | 1091 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 67 | 5 | 2050 | G | C4-N9-C1' | 5.97 | 134.27 | 126.50 |
| 73 | 8 | 72 | A | N9-C4-C5 | -5.97 | 103.41 | 105.80 |
| 76 | 9 | 330 | G | N3-C4-C5 | 5.97 | 131.59 | 128.60 |
| 67 | 5 | 2458 | C | N3-C2-O2 | -5.97 | 117.72 | 121.90 |
| 67 | 5 | 2804 | C | C2-N1-C1' | 5.97 | 125.37 | 118.80 |
| 67 | 5 | 4193 | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 67 | 5 | 418 | A | C5-C6-N1 | 5.97 | 120.68 | 117.70 |
| 67 | 5 | 1651 | G | N1-C2-N3 | 5.97 | 127.48 | 123.90 |
| 67 | 5 | 1580 | C | C5-C4-N4 | -5.96 | 116.03 | 120.20 |
| 67 | 5 | 1608 | G | C4-N9-C1' | 5.96 | 134.25 | 126.50 |
| 67 | 5 | 2419 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 67 | 5 | 4984 | C | N3-C4-C5 | 5.96 | 124.29 | 121.90 |
| 67 | 5 | 1663 | C | C5-C4-N4 | -5.96 | 116.03 | 120.20 |
| 67 | 5 | 1938 | C | C5-C4-N4 | -5.96 | 116.03 | 120.20 |
| 67 | 5 | 2419 | C | N3-C2-O2 | -5.96 | 117.73 | 121.90 |
| 67 | 5 | 4654 | C | N3-C2-O2 | -5.96 | 117.73 | 121.90 |
| 67 | 5 | 41 | C | C2-N1-C1' | 5.96 | 125.36 | 118.80 |
| 67 | 5 | 3917 | A | N1-C6-N6 | 5.96 | 122.17 | 118.60 |
| 67 | 5 | 4560 | C | C6-N1-C2 | 5.96 | 122.68 | 120.30 |
| 67 | 5 | 4716 | C | N3-C4-C5 | 5.96 | 124.28 | 121.90 |
| 76 | 9 | 1488 | C | C2-N1-C1' | 5.96 | 125.36 | 118.80 |
| 67 | 5 | 1681 | G | N3-C2-N2 | 5.96 | 124.07 | 119.90 |
| 67 | 5 | 2878 | G | C4-N9-C1' | 5.96 | 134.24 | 126.50 |
| 67 | 5 | 1931 | C | N3-C4-N4 | 5.95 | 122.17 | 118.00 |
| 67 | 5 | 2392 | C | C2-N1-C1' | 5.95 | 125.35 | 118.80 |
| 76 | 9 | 168 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 67 | 5 | 2758 | G | C4-N9-C1' | 5.95 | 134.24 | 126.50 |
| 67 | 5 | 3835 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 67 | 5 | 4510 | A | C8-N9-C1' | -5.95 | 116.99 | 127.70 |
| 76 | 9 | 1416 | C | C5-C6-N1 | 5.95 | 123.98 | 121.00 |
| 67 | 5 | 54 | G | C4-N9-C1' | 5.95 | 134.23 | 126.50 |
| 76 | 9 | 1760 | G | C5-C6-O6 | 5.95 | 132.17 | 128.60 |
| 76 | 9 | 1834 | A | C6-C5-N7 | -5.95 | 128.14 | 132.30 |
| 67 | 5 | 1879 | C | C2-N1-C1' | 5.95 | 125.34 | 118.80 |
| 76 | 9 | 480 | G | O5'-P-OP2 | -5.95 | 100.35 | 105.70 |
| 67 | 5 | 4746 | C | C2-N1-C1' | 5.94 | 125.34 | 118.80 |
| 67 | 5 | 2355 | G | N1-C2-N2 | -5.94 | 110.85 | 116.20 |
| 76 | 9 | 1566 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1628 | C | N3-C4-C5 | 5.94 | 124.28 | 121.90 |
| 76 | 9 | 1603 | G | N1-C2-N2 | -5.94 | 110.86 | 116.20 |
| 67 | 5 | 284 | G | N3-C4-C5 | -5.94 | 125.63 | 128.60 |
| 67 | 5 | 4511 | A | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 67 | 5 | 1868 | A | C5-C6-N6 | -5.93 | 118.95 | 123.70 |
| 67 | 5 | 1958 | A | N1-C6-N6 | -5.93 | 115.04 | 118.60 |
| 67 | 5 | 4291 | G | C4-N9-C1' | 5.93 | 134.21 | 126.50 |
| 67 | 5 | 4533 | A | C5-N7-C8 | -5.93 | 100.93 | 103.90 |
| 67 | 5 | 4902 | C | C2-N1-C1' | 5.93 | 125.32 | 118.80 |
| 67 | 5 | 285 | G | C2-N3-C4 | -5.93 | 108.94 | 111.90 |
| 67 | 5 | 1300 | G | N3-C4-N9 | -5.93 | 122.44 | 126.00 |
| 67 | 5 | 51 | A | C4-C5-N7 | 5.93 | 113.66 | 110.70 |
| 67 | 5 | 2435 | G | N3-C4-C5 | 5.93 | 131.56 | 128.60 |
| 67 | 5 | 3727 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |
| 55 | s | 47 | LEU | CA-CB-CG | 5.92 | 128.92 | 115.30 |
| 67 | 5 | 1888 | A | N1-C6-N6 | -5.92 | 115.05 | 118.60 |
| 67 | 5 | 2579 | G | C5-C6-O6 | 5.92 | 132.15 | 128.60 |
| 76 | 9 | 1735 | A | N1-C6-N6 | 5.92 | 122.15 | 118.60 |
| 67 | 5 | 11 | G | N3-C4-N9 | 5.92 | 129.55 | 126.00 |
| 73 | 8 | 15 | G | C4-N9-C1' | 5.92 | 134.20 | 126.50 |
| 55 | s | 155 | LEU | CA-CB-CG | 5.92 | 128.91 | 115.30 |
| 67 | 5 | 2784 | C | C6-N1-C1' | -5.92 | 113.70 | 120.80 |
| 67 | 5 | 3685 | C | C6-N1-C1' | -5.91 | 113.70 | 120.80 |
| 76 | 9 | 29 | G | C8-N9-C4 | -5.91 | 104.03 | 106.40 |
| 67 | 5 | 421 | C | N3-C4-C5 | 5.91 | 124.27 | 121.90 |
| 67 | 5 | 342 | G | N3-C4-C5 | -5.91 | 125.64 | 128.60 |
| 76 | 9 | 159 | A | N1-C6-N6 | -5.91 | 115.05 | 118.60 |
| 67 | 5 | 360 | A | C5-C6-N6 | -5.91 | 118.97 | 123.70 |
| 67 | 5 | 1283 | G | C2-N3-C4 | -5.91 | 108.95 | 111.90 |
| 73 | 8 | 39 | G | C2-N3-C4 | -5.91 | 108.95 | 111.90 |
| 67 | 5 | 1635 | C | N3-C4-C5 | 5.91 | 124.26 | 121.90 |
| 67 | 5 | 1880 | G | N1-C2-N2 | -5.91 | 110.89 | 116.20 |
| 73 | 8 | 6 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |
| 76 | 9 | 563 | G | C8-N9-C1' | -5.91 | 119.32 | 127.00 |
| 67 | 5 | 4667 | C | C2-N1-C1' | 5.90 | 125.29 | 118.80 |
| 67 | 5 | 3867 | A | C5-C6-N6 | -5.90 | 118.98 | 123.70 |
| 76 | 9 | 1083 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 76 | 9 | 1180 | C | C6-N1-C2 | 5.90 | 122.66 | 120.30 |
| 67 | 5 | 3612 | C | N3-C2-O2 | -5.90 | 117.77 | 121.90 |
| 67 | 5 | 3691 | G | C2-N3-C4 | -5.90 | 108.95 | 111.90 |
| 67 | 5 | 4671 | C | C2-N1-C1' | 5.90 | 125.29 | 118.80 |
| 76 | 9 | 604 | A | O4'-C1'-N9 | -5.90 | 103.48 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | 9 | 1181 | A | C5-C6-N6 | -5.90 | 118.98 | 123.70 |
| 67 | 5 | 4298 | A | C6-N1-C2 | -5.89 | 115.06 | 118.60 |
| 67 | 5 | 1390 | G | N1-C2-N2 | -5.89 | 110.90 | 116.20 |
| 67 | 5 | 1988 | G | C2-N3-C4 | -5.89 | 108.95 | 111.90 |
| 76 | 9 | 390 | C | C2-N1-C1' | 5.89 | 125.28 | 118.80 |
| 76 | 9 | 480 | G | N3-C4-N9 | 5.89 | 129.54 | 126.00 |
| 67 | 5 | 489 | C | N3-C4-C5 | 5.89 | 124.26 | 121.90 |
| 67 | 5 | 2392 | C | N1-C2-O2 | 5.89 | 122.43 | 118.90 |
| 67 | 5 | 2724 | G | N3-C4-C5 | 5.89 | 131.54 | 128.60 |
| 67 | 5 | 4179 | G | N7-C8-N9 | 5.89 | 116.05 | 113.10 |
| 67 | 5 | 4427 | G | N1-C2-N2 | -5.89 | 110.90 | 116.20 |
| 76 | 9 | 123 | G | C8-N9-C1' | -5.89 | 119.34 | 127.00 |
| 67 | 5 | 429 | A | C5-C6-N6 | -5.89 | 118.99 | 123.70 |
| 67 | 5 | 1546 | C | N3-C4-C5 | 5.89 | 124.25 | 121.90 |
| 67 | 5 | 4582 | C | N3-C2-O2 | -5.89 | 117.78 | 121.90 |
| 76 | 9 | 1223 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 67 | 5 | 1896 | A | C8-N9-C1' | -5.88 | 117.11 | 127.70 |
| 76 | 9 | 1603 | G | C6-C5-N7 | -5.88 | 126.87 | 130.40 |
| 16 | g | 25 | THR | CA-CB-CG2 | -5.88 | 104.17 | 112.40 |
| 67 | 5 | 422 | C | C5-C4-N4 | -5.88 | 116.08 | 120.20 |
| 67 | 5 | 1576 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 67 | 5 | 1895 | G | C8-N9-C1' | -5.88 | 119.36 | 127.00 |
| 67 | 5 | 1296 | G | O4'-C1'-N9 | 5.88 | 112.90 | 108.20 |
| 67 | 5 | 422 | C | N1-C2-O2 | 5.88 | 122.42 | 118.90 |
| 67 | 5 | 98 | A | C5-C6-N1 | 5.87 | 120.64 | 117.70 |
| 67 | 5 | 2693 | G | C4-N9-C1' | 5.87 | 134.13 | 126.50 |
| 67 | 5 | 2335 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 67 | 5 | 1654 | G | N3-C2-N2 | 5.87 | 124.01 | 119.90 |
| 67 | 5 | 2670 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 67 | 5 | 4738 | C | N3-C4-N4 | 5.87 | 122.11 | 118.00 |
| 76 | 9 | 1498 | A | C5-C6-N1 | 5.87 | 120.63 | 117.70 |
| 67 | 5 | 4510 | A | C4-N9-C1' | 5.87 | 136.86 | 126.30 |
| 67 | 5 | 1589 | C | C5-C4-N4 | -5.87 | 116.09 | 120.20 |
| 67 | 5 | 3826 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 67 | 5 | 4978 | G | N3-C2-N2 | 5.87 | 124.01 | 119.90 |
| 67 | 5 | 499 | G | N3-C2-N2 | 5.86 | 124.00 | 119.90 |
| 76 | 9 | 1294 | G | N3-C2-N2 | 5.86 | 124.00 | 119.90 |
| 67 | 5 | 1589 | C | N3-C4-C5 | 5.86 | 124.25 | 121.90 |
| 76 | 9 | 594 | A | O4'-C1'-N9 | 5.86 | 112.89 | 108.20 |
| 8 | EE | 48 | LEU | CB-CG-CD2 | -5.86 | 101.04 | 111.00 |
| 67 | 5 | 38 | A | C4-C5-C6 | 5.86 | 119.93 | 117.00 |
| 67 | 5 | 298 | G | C8-N9-C1' | -5.86 | 119.38 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 339 | C | C2-N1-C1' | 5.85 | 125.24 | 118.80 |
| 67 | 5 | 2748 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 67 | 5 | 4407 | G | C8-N9-C1' | -5.85 | 119.39 | 127.00 |
| 67 | 5 | 4528 | G | N3-C4-C5 | -5.85 | 125.67 | 128.60 |
| 76 | 9 | 909 | G | C2-N3-C4 | 5.85 | 114.83 | 111.90 |
| 73 | 8 | 45 | C | N3-C2-O2 | -5.85 | 117.81 | 121.90 |
| 76 | 9 | 1658 | G | N1-C6-O6 | 5.85 | 123.41 | 119.90 |
| 67 | 5 | 283 | G | C4-N9-C1' | 5.85 | 134.10 | 126.50 |
| 76 | 9 | 1335 | G | C4-C5-N7 | 5.85 | 113.14 | 110.80 |
| 76 | 9 | 52 | G | N3-C4-N9 | -5.84 | 122.49 | 126.00 |
| 67 | 5 | 294 | G | N9-C4-C5 | -5.84 | 103.06 | 105.40 |
| 67 | 5 | 2277 | C | C5-C4-N4 | -5.84 | 116.11 | 120.20 |
| 67 | 5 | 2627 | C | C2-N1-C1' | 5.84 | 125.22 | 118.80 |
| 67 | 5 | 4645 | C | C2-N1-C1' | 5.84 | 125.22 | 118.80 |
| 73 | 8 | 45 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 67 | 5 | 1460 | C | C5-C4-N4 | -5.84 | 116.11 | 120.20 |
| 67 | 5 | 2397 | G | C2-N3-C4 | -5.84 | 108.98 | 111.90 |
| 67 | 5 | 3901 | A | C4-N9-C1' | 5.84 | 136.81 | 126.30 |
| 67 | 5 | 4917 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 76 | 9 | 140 | U | C6-N1-C1' | -5.84 | 113.03 | 121.20 |
| 67 | 5 | 90 | G | N7-C8-N9 | 5.84 | 116.02 | 113.10 |
| 67 | 5 | 1931 | C | C5-C4-N4 | -5.84 | 116.11 | 120.20 |
| 67 | 5 | 295 | A | O4'-C1'-N9 | 5.83 | 112.87 | 108.20 |
| 67 | 5 | 1976 | G | N3-C4-C5 | 5.83 | 131.52 | 128.60 |
| 67 | 5 | 2724 | G | C2-N3-C4 | -5.83 | 108.98 | 111.90 |
| 82 | c | 39 | ARG | CG-CD-NE | 5.83 | 124.05 | 111.80 |
| 67 | 5 | 1667 | A | C5-C6-N1 | 5.83 | 120.61 | 117.70 |
| 67 | 5 | 3899 | G | C8-N9-C4 | -5.83 | 104.07 | 106.40 |
| 67 | 5 | 4278 | C | C6-N1-C1' | -5.83 | 113.81 | 120.80 |
| 67 | 5 | 4324 | A | C5-C6-N1 | 5.83 | 120.61 | 117.70 |
| 67 | 5 | 3866 | C | C6-N1-C1' | -5.83 | 113.81 | 120.80 |
| 67 | 5 | 3619 | G | N3-C4-C5 | 5.83 | 131.51 | 128.60 |
| 67 | 5 | 1064 | G | C8-N9-C1' | -5.82 | 119.43 | 127.00 |
| 67 | 5 | 1506 | G | N1-C2-N2 | -5.82 | 110.96 | 116.20 |
| 67 | 5 | 2443 | G | C6-C5-N7 | -5.82 | 126.91 | 130.40 |
| 67 | 5 | 1854 | G | C2-N3-C4 | -5.82 | 108.99 | 111.90 |
| 67 | 5 | 437 | G | C4-N9-C1' | 5.82 | 134.07 | 126.50 |
| 67 | 5 | 1553 | A | C5-C6-N6 | -5.82 | 119.04 | 123.70 |
| 76 | 9 | 1501 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 67 | 5 | 4537 | C | O4'-C1'-N1 | 5.82 | 112.86 | 108.20 |
| 76 | 9 | 674 | C | C6-N1-C2 | 5.82 | 122.63 | 120.30 |
| 4 | DD | 138 | VAL | CG1-CB-CG2 | 5.82 | 120.21 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 23 | hh | 44 | A | O5'-P-OP1 | -5.82 | 100.46 | 105.70 |
| 67 | 5 | 55 | G | C8-N9-C4 | -5.82 | 104.07 | 106.40 |
| 67 | 5 | 2282 | A | N1-C6-N6 | -5.82 | 115.11 | 118.60 |
| 67 | 5 | 3873 | G | C4-N9-C1' | 5.82 | 134.06 | 126.50 |
| 76 | 9 | 1529 | C | O4'-C1'-N1 | 5.82 | 112.85 | 108.20 |
| 67 | 5 | 1541 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 76 | 9 | 639 | C | C2-N1-C1' | 5.82 | 125.20 | 118.80 |
| 67 | 5 | 4204 | C | C6-N1-C2 | -5.81 | 117.97 | 120.30 |
| 76 | 9 | 82 | G | C4-N9-C1' | 5.81 | 134.06 | 126.50 |
| 54 | R | 173 | ARG | CA-CB-CG | 5.81 | 126.19 | 113.40 |
| 67 | 5 | 2539 | C | C6-N1-C1' | -5.81 | 113.83 | 120.80 |
| 76 | 9 | 1438 | A | N9-C4-C5 | -5.81 | 103.47 | 105.80 |
| 70 | 7 | 82 | G | C8-N9-C4 | -5.81 | 104.08 | 106.40 |
| 76 | 9 | 1294 | G | C8-N9-C1' | -5.81 | 119.45 | 127.00 |
| 67 | 5 | 3850 | C | N1-C2-O2 | 5.81 | 122.38 | 118.90 |
| 67 | 5 | 4472 | G | C8-N9-C1' | -5.81 | 119.45 | 127.00 |
| 67 | 5 | 83 | C | C5-C4-N4 | -5.80 | 116.14 | 120.20 |
| 67 | 5 | 1529 | G | N1-C2-N2 | -5.80 | 110.98 | 116.20 |
| 67 | 5 | 1541 | C | N3-C2-O2 | -5.80 | 117.84 | 121.90 |
| 67 | 5 | 4293 | U | O4'-C1'-N1 | 5.80 | 112.84 | 108.20 |
| 67 | 5 | 1608 | G | C8-N9-C1' | -5.80 | 119.46 | 127.00 |
| 67 | 5 | 4510 | A | C6-C5-N7 | -5.80 | 128.24 | 132.30 |
| 67 | 5 | 1353 | G | C8-N9-C1' | -5.80 | 119.46 | 127.00 |
| 67 | 5 | 4694 | G | C4-N9-C1' | 5.80 | 134.04 | 126.50 |
| 67 | 5 | 4979 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 67 | 5 | 1520 | C | N1-C2-O2 | 5.80 | 122.38 | 118.90 |
| 67 | 5 | 1780 | A | C5-C6-N1 | 5.80 | 120.60 | 117.70 |
| 67 | 5 | 1202 | C | N1-C1'-C2' | -5.80 | 105.62 | 112.00 |
| 67 | 5 | 4486 | C | N3-C4-N4 | 5.80 | 122.06 | 118.00 |
| 76 | 9 | 84 | A | C6-C5-N7 | -5.79 | 128.24 | 132.30 |
| 76 | 9 | 1661 | A | P-O3'-C3' | 5.79 | 126.65 | 119.70 |
| 67 | 5 | 335 | A | C5-C6-N1 | 5.79 | 120.60 | 117.70 |
| 67 | 5 | 1218 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 67 | 5 | 1895 | G | N3-C2-N2 | 5.79 | 123.95 | 119.90 |
| 67 | 5 | 2731 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 67 | 5 | 4710 | C | C2-N1-C1' | 5.79 | 125.17 | 118.80 |
| 76 | 9 | 1373 | C | C6-N1-C2 | 5.79 | 122.62 | 120.30 |
| 67 | 5 | 1271 | G | N3-C4-C5 | -5.79 | 125.70 | 128.60 |
| 67 | 5 | 2088 | A | N1-C6-N6 | 5.79 | 122.07 | 118.60 |
| 67 | 5 | 3636 | C | N3-C2-O2 | -5.79 | 117.85 | 121.90 |
| 76 | 9 | 1250 | A | N1-C6-N6 | 5.79 | 122.07 | 118.60 |
| 67 | 5 | 2746 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4550 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 67 | 5 | 1427 | A | C8-N9-C4 | 5.79 | 108.11 | 105.80 |
| 67 | 5 | 1589 | C | C6-N1-C1' | -5.79 | 113.86 | 120.80 |
| 67 | 5 | 4506 | C | C2-N1-C1' | 5.79 | 125.16 | 118.80 |
| 67 | 5 | 4176 | C | N3-C4-C5 | 5.78 | 124.21 | 121.90 |
| 76 | 9 | 1337 | C | O4'-C1'-N1 | 5.78 | 112.83 | 108.20 |
| 67 | 5 | 2438 | A | C4-C5-N7 | 5.78 | 113.59 | 110.70 |
| 67 | 5 | 2836 | A | N3-C4-C5 | 5.78 | 130.84 | 126.80 |
| 73 | 8 | 6 | C | C2-N1-C1' | 5.78 | 125.15 | 118.80 |
| 76 | 9 | 1603 | G | N9-C4-C5 | -5.78 | 103.09 | 105.40 |
| 67 | 5 | 409 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 67 | 5 | 955 | G | N3-C2-N2 | 5.77 | 123.94 | 119.90 |
| 67 | 5 | 81 | C | N3-C4-N4 | 5.77 | 122.04 | 118.00 |
| 67 | 5 | 4525 | C | C2-N1-C1' | 5.77 | 125.15 | 118.80 |
| 76 | 9 | 351 | G | N3-C4-N9 | -5.77 | 122.54 | 126.00 |
| 67 | 5 | 1371 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 67 | 5 | 4324 | A | C5-C6-N6 | -5.77 | 119.08 | 123.70 |
| 67 | 5 | 4603 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 17 | BB | 165 | ARG | CG-CD-NE | 5.77 | 123.91 | 111.80 |
| 67 | 5 | 353 | A | C4-N9-C1' | 5.77 | 136.68 | 126.30 |
| 67 | 5 | 2586 | G | O4'-C1'-N9 | -5.77 | 103.59 | 108.20 |
| 70 | 7 | 95 | C | C6-N1-C1' | -5.77 | 113.88 | 120.80 |
| 67 | 5 | 2325 | C | C2-N1-C1' | 5.76 | 125.14 | 118.80 |
| 83 | CC | 78 | LEU | CB-CG-CD2 | 5.76 | 120.80 | 111.00 |
| 67 | 5 | 1585 | C | N3-C2-O2 | -5.76 | 117.87 | 121.90 |
| 67 | 5 | 1893 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 67 | 5 | 2630 | U | P-O3'-C3' | 5.76 | 126.62 | 119.70 |
| 76 | 9 | 998 | A | N1-C6-N6 | -5.76 | 115.14 | 118.60 |
| 1 | A | 150 | LEU | CA-CB-CG | 5.76 | 128.55 | 115.30 |
| 28 | ii | 290 | TYR | CB-CG-CD2 | 5.76 | 124.46 | 121.00 |
| 67 | 5 | 1640 | C | N1-C2-O2 | 5.76 | 122.36 | 118.90 |
| 67 | 5 | 4567 | G | C8-N9-C4 | -5.76 | 104.09 | 106.40 |
| 67 | 5 | 962 | C | C6-N1-C1' | -5.76 | 113.89 | 120.80 |
| 67 | 5 | 3916 | G | N3-C4-N9 | 5.76 | 129.46 | 126.00 |
| 67 | 5 | 4701 | A | C4-N9-C1' | -5.76 | 115.93 | 126.30 |
| 76 | 9 | 1394 | G | C8-N9-C1' | -5.76 | 119.51 | 127.00 |
| 76 | 9 | 1470 | C | O4'-C1'-N1 | 5.76 | 112.81 | 108.20 |
| 67 | 5 | 301 | G | N1-C2-N2 | -5.76 | 111.02 | 116.20 |
| 67 | 5 | 3864 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 67 | 5 | 4980 | C | N3-C4-C5 | 5.76 | 124.20 | 121.90 |
| 67 | 5 | 2750 | G | N3-C2-N2 | 5.75 | 123.93 | 119.90 |
| 67 | 5 | 1183 | C | N3-C2-O2 | -5.75 | 117.87 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1308 | C | C5-C6-N1 | 5.75 | 123.88 | 121.00 |
| 67 | 5 | 4362 | A | N1-C6-N6 | -5.75 | 115.15 | 118.60 |
| 67 | 5 | 4680 | G | C8-N9-C1' | -5.75 | 119.52 | 127.00 |
| 67 | 5 | 4407 | G | C4-N9-C1' | 5.75 | 133.97 | 126.50 |
| 67 | 5 | 4583 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 67 | 5 | 3704 | U | C6-N1-C2 | -5.75 | 117.55 | 121.00 |
| 76 | 9 | 501 | C | C2-N1-C1' | 5.75 | 125.12 | 118.80 |
| 67 | 5 | 4367 | G | N1-C2-N2 | -5.75 | 111.03 | 116.20 |
| 67 | 5 | 163 | A | C4-C5-N7 | 5.74 | 113.57 | 110.70 |
| 67 | 5 | 3879 | G | C2-N3-C4 | -5.74 | 109.03 | 111.90 |
| 59 | SS | 45 | LEU | CA-CB-CG | 5.74 | 128.51 | 115.30 |
| 67 | 5 | 671 | G | N3-C4-C5 | 5.74 | 131.47 | 128.60 |
| 67 | 5 | 222 | C | C5-C4-N4 | -5.74 | 116.18 | 120.20 |
| 67 | 5 | 1896 | A | C4-N9-C1' | 5.74 | 136.63 | 126.30 |
| 67 | 5 | 4386 | C | N3-C4-N4 | -5.74 | 113.98 | 118.00 |
| 67 | 5 | 1178 | G | O4'-C1'-N9 | 5.73 | 112.79 | 108.20 |
| 67 | 5 | 1587 | G | N7-C8-N9 | 5.73 | 115.97 | 113.10 |
| 67 | 5 | 4910 | A | O4'-C1'-N9 | -5.73 | 103.61 | 108.20 |
| 76 | 9 | 989 | C | C5-C4-N4 | -5.73 | 116.19 | 120.20 |
| 21 | h | 28 | LEU | CB-CG-CD2 | -5.73 | 101.26 | 111.00 |
| 67 | 5 | 4485 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 67 | 5 | 4622 | A | C6-N1-C2 | -5.73 | 115.16 | 118.60 |
| 70 | 7 | 97 | G | C2-N3-C4 | -5.72 | 109.04 | 111.90 |
| 76 | 9 | 915 | G | C4-N9-C1' | 5.72 | 133.94 | 126.50 |
| 67 | 5 | 2429 | A | C5-C6-N1 | 5.72 | 120.56 | 117.70 |
| 67 | 5 | 4486 | C | C5-C4-N4 | -5.72 | 116.19 | 120.20 |
| 67 | 5 | 1657 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 67 | 5 | 168 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 67 | 5 | 1575 | A | C8-N9-C1' | -5.72 | 117.41 | 127.70 |
| 70 | 7 | 48 | G | C4-C5-N7 | 5.72 | 113.09 | 110.80 |
| 67 | 5 | 3691 | G | N1-C2-N2 | -5.72 | 111.05 | 116.20 |
| 67 | 5 | 23 | C | N3-C4-C5 | 5.72 | 124.19 | 121.90 |
| 67 | 5 | 968 | C | C2-N1-C1' | 5.72 | 125.09 | 118.80 |
| 76 | 9 | 82 | G | C8-N9-C1' | -5.72 | 119.57 | 127.00 |
| 67 | 5 | 56 | A | N3-C4-N9 | -5.71 | 122.83 | 127.40 |
| 67 | 5 | 221 | C | C2-N1-C1' | 5.71 | 125.09 | 118.80 |
| 67 | 5 | 2805 | C | C2-N1-C1' | 5.71 | 125.09 | 118.80 |
| 67 | 5 | 3866 | C | C6-N1-C2 | -5.71 | 118.01 | 120.30 |
| 67 | 5 | 4669 | A | C5-C6-N1 | 5.71 | 120.56 | 117.70 |
| 76 | 9 | 1250 | A | C8-N9-C1' | -5.71 | 117.41 | 127.70 |
| 67 | 5 | 2579 | G | C2-N3-C4 | -5.71 | 109.04 | 111.90 |
| 76 | 9 | 948 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4434 | C | N1-C2-O2 | 5.71 | 122.33 | 118.90 |
| 67 | 5 | 977 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 67 | 5 | 3859 | G | C8-N9-C1' | -5.71 | 119.58 | 127.00 |
| 67 | 5 | 3871 | A | C8-N9-C1' | -5.71 | 117.42 | 127.70 |
| 67 | 5 | 4305 | G | N7-C8-N9 | 5.71 | 115.95 | 113.10 |
| 73 | 8 | 125 | C | O4'-C1'-N1 | 5.71 | 112.77 | 108.20 |
| 67 | 5 | 4291 | G | C8-N9-C1' | -5.71 | 119.58 | 127.00 |
| 67 | 5 | 2467 | U | O4'-C1'-N1 | 5.70 | 112.76 | 108.20 |
| 67 | 5 | 105 | A | N9-C4-C5 | -5.70 | 103.52 | 105.80 |
| 67 | 5 | 1929 | A | C4-N9-C1' | 5.70 | 136.56 | 126.30 |
| 76 | 9 | 1658 | G | C5-C6-O6 | -5.70 | 125.18 | 128.60 |
| 67 | 5 | 4878 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 67 | 5 | 41 | C | N3-C4-C5 | 5.70 | 124.18 | 121.90 |
| 67 | 5 | 3685 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 67 | 5 | 3746 | A | C5-C6-N6 | -5.70 | 119.14 | 123.70 |
| 67 | 5 | 4448 | G | N3-C4-C5 | 5.70 | 131.45 | 128.60 |
| 67 | 5 | 23 | C | C5-C4-N4 | -5.70 | 116.21 | 120.20 |
| 67 | 5 | 106 | A | C4-C5-C6 | 5.70 | 119.85 | 117.00 |
| 67 | 5 | 4915 | G | N3-C4-C5 | 5.69 | 131.45 | 128.60 |
| 67 | 5 | 969 | C | C6-N1-C2 | -5.69 | 118.02 | 120.30 |
| 67 | 5 | 3748 | A | N1-C2-N3 | 5.69 | 132.15 | 129.30 |
| 67 | 5 | 4171 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 28 | ii | 232 | PHE | CB-CG-CD2 | -5.69 | 116.82 | 120.80 |
| 67 | 5 | 105 | A | C5-N7-C8 | -5.69 | 101.06 | 103.90 |
| 67 | 5 | 2074 | C | N3-C4-C5 | 5.69 | 124.17 | 121.90 |
| 76 | 9 | 47 | G | C2-N3-C4 | -5.69 | 109.06 | 111.90 |
| 67 | 5 | 101 | A | N9-C4-C5 | -5.69 | 103.53 | 105.80 |
| 67 | 5 | 1920 | C | C6-N1-C1' | -5.68 | 113.98 | 120.80 |
| 67 | 5 | 1983 | A | O4'-C1'-N9 | 5.68 | 112.75 | 108.20 |
| 76 | 9 | 1055 | A | C4-C5-N7 | 5.68 | 113.54 | 110.70 |
| 67 | 5 | 4193 | C | C5-C4-N4 | -5.68 | 116.22 | 120.20 |
| 67 | 5 | 4710 | C | N3-C2-O2 | -5.68 | 117.92 | 121.90 |
| 67 | 5 | 1880 | G | C4-N9-C1' | 5.68 | 133.88 | 126.50 |
| 73 | 8 | 125 | C | N1-C1'-C2' | 5.68 | 121.38 | 114.00 |
| 73 | 8 | 135 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 76 | 9 | 639 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 67 | 5 | 18 | C | C2-N1-C1' | 5.68 | 125.05 | 118.80 |
| 67 | 5 | 2815 | A | C8-N9-C1' | -5.68 | 117.48 | 127.70 |
| 67 | 5 | 148 | A | N1-C6-N6 | 5.68 | 122.00 | 118.60 |
| 67 | 5 | 2051 | C | C5-C4-N4 | -5.68 | 116.23 | 120.20 |
| 67 | 5 | 3929 | G | C8-N9-C1' | -5.68 | 119.62 | 127.00 |
| 76 | 9 | 11 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | 9 | 1695 | A | N1-C6-N6 | 5.68 | 122.01 | 118.60 |
| 67 | 5 | 945 | U | O4'-C1'-N1 | 5.67 | 112.74 | 108.20 |
| 67 | 5 | 4230 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 67 | 5 | 4631 | G | N3-C4-N9 | 5.67 | 129.41 | 126.00 |
| 76 | 9 | 1060 | A | O4'-C1'-N9 | 5.67 | 112.74 | 108.20 |
| 67 | 5 | 1830 | G | C4-N9-C1' | 5.67 | 133.88 | 126.50 |
| 67 | 5 | 3857 | G | N3-C2-N2 | 5.67 | 123.87 | 119.90 |
| 67 | 5 | 651 | C | C2-N1-C1' | 5.67 | 125.04 | 118.80 |
| 67 | 5 | 713 | C | N3-C2-O2 | -5.67 | 117.93 | 121.90 |
| 67 | 5 | 4549 | G | N3-C2-N2 | 5.67 | 123.87 | 119.90 |
| 76 | 9 | 1257 | G | C4-N9-C1' | -5.67 | 119.13 | 126.50 |
| 67 | 5 | 1585 | C | O4'-C1'-N1 | 5.67 | 112.73 | 108.20 |
| 67 | 5 | 1627 | G | C6-C5-N7 | -5.67 | 127.00 | 130.40 |
| 76 | 9 | 504 | G | N3-C2-N2 | 5.67 | 123.87 | 119.90 |
| 67 | 5 | 4415 | A | N9-C1'-C2' | -5.67 | 105.77 | 112.00 |
| 67 | 5 | 90 | G | C4-N9-C1' | 5.66 | 133.86 | 126.50 |
| 76 | 9 | 1247 | C | O4'-C1'-N1 | -5.66 | 103.67 | 108.20 |
| 67 | 5 | 2509 | C | C6-N1-C1' | -5.66 | 114.01 | 120.80 |
| 67 | 5 | 1633 | G | P-O3'-C3' | 5.66 | 126.49 | 119.70 |
| 67 | 5 | 1660 | U | O4'-C1'-N1 | 5.66 | 112.73 | 108.20 |
| 67 | 5 | 21 | G | N3-C2-N2 | 5.66 | 123.86 | 119.90 |
| 67 | 5 | 1506 | G | N3-C2-N2 | 5.66 | 123.86 | 119.90 |
| 67 | 5 | 3891 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 76 | 9 | 1425 | G | C4-N9-C1' | 5.66 | 133.85 | 126.50 |
| 67 | 5 | 1843 | A | C5-C6-N1 | 5.66 | 120.53 | 117.70 |
| 76 | 9 | 1327 | G | O5'-P-OP2 | -5.66 | 100.61 | 105.70 |
| 67 | 5 | 336 | A | C6-N1-C2 | -5.65 | 115.21 | 118.60 |
| 67 | 5 | 1899 | G | C6-C5-N7 | -5.65 | 127.01 | 130.40 |
| 73 | 8 | 41 | A | N3-C4-N9 | -5.65 | 122.88 | 127.40 |
| 67 | 5 | 294 | G | N3-C2-N2 | 5.65 | 123.86 | 119.90 |
| 67 | 5 | 3632 | C | C2-N1-C1' | 5.65 | 125.02 | 118.80 |
| 67 | 5 | 4211 | C | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 72 | Y | 94 | THR | CA-CB-CG2 | -5.65 | 104.49 | 112.40 |
| 67 | 5 | 2789 | A | N9-C4-C5 | -5.65 | 103.54 | 105.80 |
| 67 | 5 | 4363 | A | C5-C6-N6 | -5.65 | 119.18 | 123.70 |
| 67 | 5 | 4286 | C | C2-N1-C1' | 5.65 | 125.01 | 118.80 |
| 67 | 5 | 54 | G | N1-C2-N2 | -5.65 | 111.12 | 116.20 |
| 67 | 5 | 3834 | C | C2-N1-C1' | 5.65 | 125.01 | 118.80 |
| 67 | 5 | 263 | G | C4-N9-C1' | 5.64 | 133.84 | 126.50 |
| 76 | 9 | 613 | G | C8-N9-C4 | -5.64 | 104.14 | 106.40 |
| 76 | 9 | 1610 | G | C4-N9-C1' | 5.64 | 133.84 | 126.50 |
| 67 | 5 | 4525 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 73 | 8 | 32 | C | N1-C2-O2 | 5.64 | 122.29 | 118.90 |
| 60 | T | 145 | GLY | N-CA-C | 5.64 | 127.20 | 113.10 |
| 76 | 9 | 603 | C | C6-N1-C2 | 5.64 | 122.56 | 120.30 |
| 67 | 5 | 2068 | C | C5-C6-N1 | 5.64 | 123.82 | 121.00 |
| 11 | E | 128 | LEU | CB-CG-CD2 | -5.64 | 101.42 | 111.00 |
| 67 | 5 | 41 | C | C5-C4-N4 | -5.64 | 116.25 | 120.20 |
| 67 | 5 | 1234 | G | C2-N3-C4 | -5.64 | 109.08 | 111.90 |
| 67 | 5 | 1541 | C | C5-C4-N4 | -5.64 | 116.25 | 120.20 |
| 67 | 5 | 1510 | G | C8-N9-C1' | -5.64 | 119.67 | 127.00 |
| 67 | 5 | 1738 | A | C5-C6-N6 | -5.64 | 119.19 | 123.70 |
| 67 | 5 | 3901 | A | C6-C5-N7 | -5.64 | 128.35 | 132.30 |
| 76 | 9 | 624 | C | C6-N1-C2 | -5.64 | 118.05 | 120.30 |
| 67 | 5 | 1314 | C | O4'-C1'-N1 | 5.63 | 112.71 | 108.20 |
| 67 | 5 | 1321 | G | N1-C2-N2 | -5.63 | 111.13 | 116.20 |
| 67 | 5 | 2896 | G | C8-N9-C4 | -5.63 | 104.15 | 106.40 |
| 67 | 5 | 4091 | G | N3-C4-C5 | -5.63 | 125.78 | 128.60 |
| 67 | 5 | 4502 | C | O4'-C1'-N1 | 5.63 | 112.71 | 108.20 |
| 67 | 5 | 4681 | A | N9-C4-C5 | -5.63 | 103.55 | 105.80 |
| 67 | 5 | 352 | G | C6-C5-N7 | -5.63 | 127.02 | 130.40 |
| 67 | 5 | 364 | G | C6-C5-N7 | -5.63 | 127.02 | 130.40 |
| 67 | 5 | 4517 | A | C8-N9-C4 | -5.63 | 103.55 | 105.80 |
| 67 | 5 | 166 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 67 | 5 | 1373 | A | C5-C6-N6 | -5.63 | 119.20 | 123.70 |
| 67 | 5 | 4189 | U | N3-C4-O4 | 5.63 | 123.34 | 119.40 |
| 76 | 9 | 547 | G | C8-N9-C1' | -5.63 | 119.68 | 127.00 |
| 67 | 5 | 1607 | C | C2-N1-C1' | 5.63 | 124.99 | 118.80 |
| 67 | 5 | 1654 | G | N9-C4-C5 | -5.63 | 103.15 | 105.40 |
| 67 | 5 | 3858 | C | C2-N1-C1' | 5.63 | 124.99 | 118.80 |
| 76 | 9 | 35 | C | N3-C4-C5 | 5.63 | 124.15 | 121.90 |
| 67 | 5 | 1191 | C | C5-C4-N4 | 5.63 | 124.14 | 120.20 |
| 67 | 5 | 2543 | A | N1-C6-N6 | 5.63 | 121.97 | 118.60 |
| 67 | 5 | 3617 | G | N3-C4-C5 | 5.63 | 131.41 | 128.60 |
| 67 | 5 | 1358 | G | O4'-C1'-N9 | -5.62 | 103.70 | 108.20 |
| 67 | 5 | 1998 | A | O4'-C1'-N9 | -5.62 | 103.70 | 108.20 |
| 67 | 5 | 4945 | G | N1-C2-N2 | -5.62 | 111.14 | 116.20 |
| 73 | 8 | 47 | C | C2-N1-C1' | 5.62 | 124.99 | 118.80 |
| 67 | 5 | 942 | G | N1-C2-N2 | -5.62 | 111.14 | 116.20 |
| 67 | 5 | 1515 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 67 | 5 | 2022 | C | N3-C4-C5 | 5.62 | 124.15 | 121.90 |
| 67 | 5 | 2672 | C | C2-N1-C1' | 5.62 | 124.98 | 118.80 |
| 67 | 5 | 3911 | C | C5-C4-N4 | -5.62 | 116.26 | 120.20 |
| 67 | 5 | 719 | C | C2-N1-C1' | 5.62 | 124.98 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1812 | C | N1-C2-O2 | 5.62 | 122.27 | 118.90 |
| 67 | 5 | 2754 | G | C2-N3-C4 | -5.62 | 109.09 | 111.90 |
| 67 | 5 | 3871 | A | C5-C6-N1 | 5.62 | 120.51 | 117.70 |
| 76 | 9 | 347 | G | N1-C2-N2 | 5.62 | 121.26 | 116.20 |
| 67 | 5 | 4516 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 67 | 5 | 4917 | C | C6-N1-C1' | -5.61 | 114.06 | 120.80 |
| 67 | 5 | 1306 | C | C6-N1-C1' | -5.61 | 114.07 | 120.80 |
| 67 | 5 | 1764 | G | C4-N9-C1' | 5.61 | 133.79 | 126.50 |
| 67 | 5 | 1895 | G | C4-N9-C1' | 5.61 | 133.79 | 126.50 |
| 67 | 5 | 2337 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 73 | 8 | 28 | C | C2-N1-C1' | 5.61 | 124.97 | 118.80 |
| 67 | 5 | 1323 | A | C5-N7-C8 | -5.61 | 101.10 | 103.90 |
| 67 | 5 | 1812 | C | C5-C4-N4 | -5.61 | 116.27 | 120.20 |
| 73 | 8 | 44 | A | C6-C5-N7 | -5.61 | 128.38 | 132.30 |
| 34 | k | 64 | LEU | CA-CB-CG | 5.61 | 128.19 | 115.30 |
| 76 | 9 | 1740 | C | C5-C4-N4 | -5.61 | 116.28 | 120.20 |
| 76 | 9 | 1019 | C | C6-N1-C1' | -5.60 | 114.08 | 120.80 |
| 67 | 5 | 298 | G | C4-N9-C1' | 5.60 | 133.78 | 126.50 |
| 67 | 5 | 955 | G | C4-N9-C1' | 5.60 | 133.78 | 126.50 |
| 67 | 5 | 1586 | G | C8-N9-C4 | -5.60 | 104.16 | 106.40 |
| 67 | 5 | 1739 | G | C8-N9-C1' | -5.60 | 119.72 | 127.00 |
| 67 | 5 | 2071 | A | C5-C6-N1 | 5.60 | 120.50 | 117.70 |
| 67 | 5 | 2889 | G | C4-N9-C1' | 5.60 | 133.78 | 126.50 |
| 67 | 5 | 4479 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 67 | 5 | 4291 | G | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 67 | 5 | 4533 | A | N9-C4-C5 | -5.60 | 103.56 | 105.80 |
| 67 | 5 | 4640 | C | C5-C4-N4 | -5.60 | 116.28 | 120.20 |
| 76 | 9 | 329 | G | C8-N9-C1' | -5.60 | 119.72 | 127.00 |
| 67 | 5 | 1924 | C | C6-N1-C1' | -5.60 | 114.08 | 120.80 |
| 67 | 5 | 38 | A | N3-C4-N9 | 5.59 | 131.88 | 127.40 |
| 67 | 5 | 386 | A | C4-C5-N7 | 5.59 | 113.50 | 110.70 |
| 67 | 5 | 418 | A | N1-C2-N3 | 5.59 | 132.10 | 129.30 |
| 67 | 5 | 4671 | C | C5-C4-N4 | -5.59 | 116.28 | 120.20 |
| 67 | 5 | 1484 | G | N3-C4-N9 | 5.59 | 129.36 | 126.00 |
| 67 | 5 | 1537 | A | C5-C6-N1 | 5.59 | 120.50 | 117.70 |
| 67 | 5 | 1675 | C | C6-N1-C1' | -5.59 | 114.09 | 120.80 |
| 67 | 5 | 2081 | C | C2-N1-C1' | 5.59 | 124.95 | 118.80 |
| 67 | 5 | 2282 | A | C8-N9-C4 | -5.59 | 103.56 | 105.80 |
| 67 | 5 | 3820 | G | C4-N9-C1' | 5.59 | 133.77 | 126.50 |
| 76 | 9 | 1414 | A | O4'-C1'-N9 | -5.59 | 103.73 | 108.20 |
| 67 | 5 | 364 | G | N9-C4-C5 | -5.59 | 103.16 | 105.40 |
| 67 | 5 | 3871 | A | N1-C2-N3 | 5.59 | 132.09 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4949 | G | N3-C2-N2 | -5.59 | 115.99 | 119.90 |
| 67 | 5 | 364 | G | O4'-C1'-N9 | 5.59 | 112.67 | 108.20 |
| 67 | 5 | 100 | C | N3-C4-C5 | 5.59 | 124.14 | 121.90 |
| 67 | 5 | 2443 | G | N3-C4-C5 | -5.59 | 125.81 | 128.60 |
| 73 | 8 | 26 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 76 | 9 | 1014 | G | N9-C4-C5 | -5.59 | 103.17 | 105.40 |
| 67 | 5 | 656 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 67 | 5 | 4213 | A | C4-N9-C1' | 5.58 | 136.35 | 126.30 |
| 67 | 5 | 4503 | A | C5-C6-N1 | 5.58 | 120.49 | 117.70 |
| 67 | 5 | 1321 | G | C4-N9-C1' | 5.58 | 133.76 | 126.50 |
| 67 | 5 | 1872 | G | N1-C2-N2 | -5.58 | 111.18 | 116.20 |
| 67 | 5 | 1890 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 76 | 9 | 1262 | C | O4'-C1'-N1 | 5.58 | 112.67 | 108.20 |
| 67 | 5 | 1458 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 67 | 5 | 2355 | G | N3-C2-N2 | 5.58 | 123.81 | 119.90 |
| 67 | 5 | 352 | G | C4-C5-N7 | 5.58 | 113.03 | 110.80 |
| 67 | 5 | 2853 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 67 | 5 | 3924 | C | C5-C4-N4 | -5.58 | 116.30 | 120.20 |
| 67 | 5 | 3924 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 76 | 9 | 1250 | A | C4-N9-C1' | 5.58 | 136.34 | 126.30 |
| 67 | 5 | 1218 | G | C4-N9-C1' | -5.58 | 119.25 | 126.50 |
| 67 | 5 | 1329 | G | C8-N9-C1' | -5.58 | 119.75 | 127.00 |
| 67 | 5 | 4631 | G | C4-N9-C1' | 5.58 | 133.75 | 126.50 |
| 76 | 9 | 1205 | C | N3-C2-O2 | -5.58 | 118.00 | 121.90 |
| 76 | 9 | 1223 | A | N9-C4-C5 | -5.58 | 103.57 | 105.80 |
| 76 | 9 | 1275 | G | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 67 | 5 | 1816 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 67 | 5 | 3816 | A | C8-N9-C4 | -5.57 | 103.57 | 105.80 |
| 67 | 5 | 5050 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 67 | 5 | 923 | C | N3-C4-C5 | 5.57 | 124.13 | 121.90 |
| 67 | 5 | 1451 | G | C8-N9-C4 | -5.57 | 104.17 | 106.40 |
| 67 | 5 | 4380 | A | C5-C6-N6 | -5.57 | 119.24 | 123.70 |
| 76 | 9 | 1501 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 67 | 5 | 1920 | C | C2-N1-C1' | 5.57 | 124.93 | 118.80 |
| 67 | 5 | 81 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 67 | 5 | 1507 | C | C5-C6-N1 | 5.57 | 123.78 | 121.00 |
| 67 | 5 | 1632 | A | O4'-C1'-N9 | 5.57 | 112.66 | 108.20 |
| 67 | 5 | 4682 | U | O4'-C1'-N1 | 5.57 | 112.65 | 108.20 |
| 67 | 5 | 4969 | C | C6-N1-C2 | -5.57 | 118.07 | 120.30 |
| 73 | 8 | 148 | A | C6-N1-C2 | -5.57 | 115.26 | 118.60 |
| 76 | 9 | 1389 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 67 | 5 | 4681 | A | N1-C6-N6 | 5.56 | 121.94 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | 9 | 1856 | C | C5-C4-N4 | -5.56 | 116.31 | 120.20 |
| 67 | 5 | 2577 | C | N3-C4-C5 | 5.56 | 124.12 | 121.90 |
| 67 | 5 | 4186 | A | N1-C2-N3 | 5.56 | 132.08 | 129.30 |
| 67 | 5 | 4279 | A | C4-C5-N7 | 5.56 | 113.48 | 110.70 |
| 73 | 8 | 47 | C | N3-C4-N4 | 5.56 | 121.89 | 118.00 |
| 67 | 5 | 1065 | G | C5-C6-O6 | 5.56 | 131.94 | 128.60 |
| 67 | 5 | 1794 | A | C4-N9-C1' | 5.56 | 136.30 | 126.30 |
| 67 | 5 | 2379 | A | N9-C4-C5 | -5.56 | 103.58 | 105.80 |
| 73 | 8 | 28 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 73 | 8 | 44 | A | C4-C5-N7 | 5.56 | 113.48 | 110.70 |
| 76 | 9 | 140 | U | C5-C6-N1 | 5.56 | 125.48 | 122.70 |
| 56 | RR | 60 | ARG | CA-CB-CG | 5.55 | 125.62 | 113.40 |
| 67 | 5 | 1575 | A | C4-N9-C1' | 5.55 | 136.30 | 126.30 |
| 67 | 5 | 1663 | C | N3-C4-N4 | 5.55 | 121.89 | 118.00 |
| 67 | 5 | 2591 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 67 | 5 | 3774 | A | C6-C5-N7 | -5.55 | 128.41 | 132.30 |
| 67 | 5 | 4523 | A | N1-C6-N6 | -5.55 | 115.27 | 118.60 |
| 76 | 9 | 473 | A | C5-C6-N1 | 5.55 | 120.48 | 117.70 |
| 76 | 9 | 1216 | C | C6-N1-C1' | 5.55 | 127.47 | 120.80 |
| 67 | 5 | 1502 | G | N3-C4-C5 | 5.55 | 131.38 | 128.60 |
| 17 | BB | 62 | LEU | CB-CG-CD2 | -5.55 | 101.56 | 111.00 |
| 42 | N | 14 | LYS | CD-CE-NZ | 5.55 | 124.47 | 111.70 |
| 67 | 5 | 1739 | G | N3-C4-N9 | 5.55 | 129.33 | 126.00 |
| 67 | 5 | 4310 | A | C5-C6-N1 | 5.55 | 120.48 | 117.70 |
| 76 | 9 | 1610 | G | N3-C4-N9 | 5.55 | 129.33 | 126.00 |
| 67 | 5 | 284 | G | N3-C4-N9 | 5.55 | 129.33 | 126.00 |
| 67 | 5 | 2050 | G | C8-N9-C1' | -5.55 | 119.79 | 127.00 |
| 67 | 5 | 4868 | G | C8-N9-C4 | -5.55 | 104.18 | 106.40 |
| 67 | 5 | 1967 | A | N1-C6-N6 | 5.55 | 121.93 | 118.60 |
| 76 | 9 | 1354 | G | N3-C2-N2 | 5.55 | 123.78 | 119.90 |
| 67 | 5 | 234 | G | N3-C4-C5 | 5.55 | 131.37 | 128.60 |
| 67 | 5 | 1316 | G | N1-C2-N2 | -5.55 | 111.21 | 116.20 |
| 67 | 5 | 1890 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 67 | 5 | 3704 | U | N1-C2-O2 | -5.55 | 118.92 | 122.80 |
| 67 | 5 | 4091 | G | N3-C4-N9 | 5.55 | 129.33 | 126.00 |
| 67 | 5 | 4444 | C | C2-N1-C1' | 5.55 | 124.90 | 118.80 |
| 76 | 9 | 659 | G | C4-N9-C1' | 5.55 | 133.71 | 126.50 |
| 76 | 9 | 1618 | C | O5'-P-OP1 | -5.55 | 100.71 | 105.70 |
| 67 | 5 | 1455 | G | C4-N9-C1' | 5.54 | 133.71 | 126.50 |
| 67 | 5 | 409 | G | C8-N9-C4 | -5.54 | 104.18 | 106.40 |
| 67 | 5 | 1670 | G | C8-N9-C1' | -5.54 | 119.79 | 127.00 |
| 67 | 5 | 4618 | G | N7-C8-N9 | 5.54 | 115.87 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1350 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 73 | 8 | 103 | A | C5-N7-C8 | -5.54 | 101.13 | 103.90 |
| 76 | 9 | 391 | C | C6-N1-C1' | -5.54 | 114.15 | 120.80 |
| 67 | 5 | 382 | G | C8-N9-C1' | -5.54 | 119.80 | 127.00 |
| 67 | 5 | 1910 | G | C8-N9-C1' | -5.54 | 119.80 | 127.00 |
| 67 | 5 | 4384 | U | C5-C4-O4 | -5.54 | 122.58 | 125.90 |
| 67 | 5 | 4487 | A | C5-C6-N6 | -5.54 | 119.27 | 123.70 |
| 67 | 5 | 1404 | G | N3-C4-N9 | -5.54 | 122.68 | 126.00 |
| 67 | 5 | 3612 | C | C2-N1-C1' | 5.54 | 124.89 | 118.80 |
| 67 | 5 | 4124 | G | C4-N9-C1' | 5.54 | 133.70 | 126.50 |
| 76 | 9 | 1464 | C | C2-N1-C1' | -5.54 | 112.71 | 118.80 |
| 67 | 5 | 2410 | C | N1-C2-O2 | 5.54 | 122.22 | 118.90 |
| 76 | 9 | 1798 | C | C2-N1-C1' | 5.54 | 124.89 | 118.80 |
| 24 | bb | 63 | LEU | CB-CG-CD2 | -5.53 | 101.59 | 111.00 |
| 67 | 5 | 1397 | A | C5-C6-N1 | 5.53 | 120.47 | 117.70 |
| 67 | 5 | 4155 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 21 | h | 87 | LYS | CD-CE-NZ | -5.53 | 98.98 | 111.70 |
| 67 | 5 | 1274 | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 67 | 5 | 4427 | G | C4-N9-C1' | 5.53 | 133.69 | 126.50 |
| 67 | 5 | 2302 | C | C2-N1-C1' | 5.53 | 124.88 | 118.80 |
| 67 | 5 | 1795 | A | C5-C6-N1 | 5.53 | 120.46 | 117.70 |
| 76 | 9 | 1755 | C | N1-C2-O2 | 5.53 | 122.22 | 118.90 |
| 67 | 5 | 1373 | A | C8-N9-C1' | -5.53 | 117.75 | 127.70 |
| 67 | 5 | 1520 | C | C5-C4-N4 | -5.53 | 116.33 | 120.20 |
| 67 | 5 | 1878 | G | C8-N9-C4 | -5.53 | 104.19 | 106.40 |
| 67 | 5 | 4749 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |
| 67 | 5 | 707 | C | N1-C2-O2 | 5.52 | 122.21 | 118.90 |
| 67 | 5 | 4631 | G | C6-C5-N7 | -5.52 | 127.09 | 130.40 |
| 70 | 7 | 57 | C | C6-N1-C1' | -5.52 | 114.17 | 120.80 |
| 67 | 5 | 2423 | A | N1-C6-N6 | 5.52 | 121.91 | 118.60 |
| 67 | 5 | 4560 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |
| 70 | 7 | 36 | C | C2-N1-C1' | 5.52 | 124.87 | 118.80 |
| 67 | 5 | 285 | G | N1-C2-N2 | -5.52 | 111.23 | 116.20 |
| 67 | 5 | 1503 | A | O4'-C1'-N9 | 5.52 | 112.61 | 108.20 |
| 67 | 5 | 2025 | A | C4-C5-C6 | -5.52 | 114.24 | 117.00 |
| 67 | 5 | 323 | C | C2-N1-C1' | 5.52 | 124.87 | 118.80 |
| 67 | 5 | 3646 | A | N1-C6-N6 | 5.51 | 121.91 | 118.60 |
| 67 | 5 | 1322 | A | O4'-C1'-N9 | -5.51 | 103.79 | 108.20 |
| 76 | 9 | 293 | C | O4'-C1'-N1 | 5.51 | 112.61 | 108.20 |
| 67 | 5 | 1887 | G | C4-N9-C1' | 5.51 | 133.66 | 126.50 |
| 67 | 5 | 5008 | C | C5-C4-N4 | -5.51 | 116.34 | 120.20 |
| 76 | 9 | 911 | C | N3-C4-C5 | 5.51 | 124.11 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 240 | G | C4-N9-C1' | 5.51 | 133.66 | 126.50 |
| 76 | 9 | 223 | C | C2-N1-C1' | 5.51 | 124.86 | 118.80 |
| 76 | 9 | 1793 | A | C5-C6-N1 | 5.51 | 120.45 | 117.70 |
| 67 | 5 | 2318 | G | N1-C2-N2 | -5.51 | 111.24 | 116.20 |
| 67 | 5 | 3864 | C | N3-C4-C5 | 5.51 | 124.10 | 121.90 |
| 73 | 8 | 13 | G | N1-C2-N3 | 5.51 | 127.20 | 123.90 |
| 67 | 5 | 4316 | G | C8-N9-C4 | -5.51 | 104.20 | 106.40 |
| 76 | 9 | 41 | G | O4'-C1'-N9 | 5.51 | 112.61 | 108.20 |
| 67 | 5 | 1982 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 67 | 5 | 2051 | C | C2-N1-C1' | 5.50 | 124.86 | 118.80 |
| 67 | 5 | 2420 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 67 | 5 | 4097 | G | N3-C4-C5 | 5.50 | 131.35 | 128.60 |
| 67 | 5 | 385 | A | O4'-C1'-N9 | 5.50 | 112.60 | 108.20 |
| 67 | 5 | 2332 | A | C5-N7-C8 | -5.50 | 101.15 | 103.90 |
| 67 | 5 | 2511 | A | C8-N9-C4 | -5.50 | 103.60 | 105.80 |
| 76 | 9 | 1860 | A | C6-N1-C2 | -5.50 | 115.30 | 118.60 |
| 67 | 5 | 303 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 67 | 5 | 408 | A | N7-C8-N9 | 5.50 | 116.55 | 113.80 |
| 67 | 5 | 1404 | G | N3-C4-C5 | 5.50 | 131.35 | 128.60 |
| 67 | 5 | 2878 | G | N3-C2-N2 | 5.50 | 123.75 | 119.90 |
| 67 | 5 | 3871 | A | C4-N9-C1' | 5.50 | 136.20 | 126.30 |
| 67 | 5 | 4195 | G | C4-N9-C1' | 5.50 | 133.65 | 126.50 |
| 73 | 8 | 135 | C | C2-N1-C1' | 5.50 | 124.85 | 118.80 |
| 76 | 9 | 429 | C | N1-C2-O2 | 5.50 | 122.20 | 118.90 |
| 67 | 5 | 1384 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 17 | BB | 228 | LEU | CA-CB-CG | 5.50 | 127.94 | 115.30 |
| 67 | 5 | 1887 | G | N1-C2-N2 | -5.50 | 111.25 | 116.20 |
| 67 | 5 | 2036 | C | C2-N1-C1' | 5.50 | 124.84 | 118.80 |
| 67 | 5 | 2715 | G | C2-N3-C4 | -5.50 | 109.15 | 111.90 |
| 67 | 5 | 4497 | U | O4'-C1'-N1 | 5.50 | 112.60 | 108.20 |
| 67 | 5 | 4764 | A | C8-N9-C4 | 5.50 | 108.00 | 105.80 |
| 67 | 5 | 4942 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 76 | 9 | 319 | C | C6-N1-C1' | 5.50 | 127.39 | 120.80 |
| 67 | 5 | 2793 | G | C2-N3-C4 | -5.50 | 109.15 | 111.90 |
| 67 | 5 | 3719 | A | C5-C6-N6 | -5.50 | 119.30 | 123.70 |
| 76 | 9 | 347 | G | N3-C4-C5 | 5.50 | 131.35 | 128.60 |
| 67 | 5 | 452 | A | N1-C6-N6 | 5.49 | 121.90 | 118.60 |
| 67 | 5 | 2435 | G | N3-C4-N9 | -5.49 | 122.70 | 126.00 |
| 67 | 5 | 2438 | A | C5-N7-C8 | -5.49 | 101.15 | 103.90 |
| 67 | 5 | 3923 | A | C5-C6-N1 | 5.49 | 120.45 | 117.70 |
| 67 | 5 | 4485 | C | N1-C2-O2 | 5.49 | 122.20 | 118.90 |
| 67 | 5 | 707 | C | N3-C2-O2 | -5.49 | 118.06 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 928 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 76 | 9 | 1828 | C | N3-C4-C5 | 5.49 | 124.10 | 121.90 |
| 67 | 5 | 1342 | A | C5-N7-C8 | -5.49 | 101.16 | 103.90 |
| 67 | 5 | 1898 | C | N3-C4-N4 | 5.49 | 121.84 | 118.00 |
| 67 | 5 | 4527 | G | C4-N9-C1' | 5.49 | 133.64 | 126.50 |
| 73 | 8 | 10 | G | C6-C5-N7 | -5.49 | 127.11 | 130.40 |
| 76 | 9 | 1215 | C | N3-C4-C5 | -5.49 | 119.70 | 121.90 |
| 67 | 5 | 437 | G | C8-N9-C1' | -5.49 | 119.87 | 127.00 |
| 67 | 5 | 2001 | G | C4-N9-C1' | -5.49 | 119.37 | 126.50 |
| 76 | 9 | 1806 | A | C5-C6-N6 | -5.49 | 119.31 | 123.70 |
| 76 | 9 | 11 | A | N1-C6-N6 | 5.48 | 121.89 | 118.60 |
| 76 | 9 | 853 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 67 | 5 | 1064 | G | N3-C4-C5 | -5.48 | 125.86 | 128.60 |
| 67 | 5 | 1629 | G | C4-N9-C1' | 5.48 | 133.63 | 126.50 |
| 67 | 5 | 4183 | G | C8-N9-C1' | 5.48 | 134.13 | 127.00 |
| 70 | 7 | 34 | C | C5-C4-N4 | -5.48 | 116.36 | 120.20 |
| 76 | 9 | 1580 | A | C8-N9-C4 | -5.48 | 103.61 | 105.80 |
| 76 | 9 | 1715 | A | C4-C5-N7 | 5.48 | 113.44 | 110.70 |
| 50 | PP | 40 | ARG | NE-CZ-NH2 | -5.48 | 117.56 | 120.30 |
| 67 | 5 | 1352 | C | N3-C4-C5 | 5.48 | 124.09 | 121.90 |
| 67 | 5 | 2878 | G | C4-C5-N7 | 5.48 | 112.99 | 110.80 |
| 67 | 5 | 1283 | G | N3-C4-N9 | -5.48 | 122.71 | 126.00 |
| 67 | 5 | 2351 | C | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 67 | 5 | 3934 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 76 | 9 | 1852 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 42 | N | 22 | LEU | CB-CG-CD2 | -5.48 | 101.69 | 111.00 |
| 67 | 5 | 285 | G | C5-C6-O6 | 5.47 | 131.88 | 128.60 |
| 72 | Y | 113 | LYS | CA-CB-CG | 5.47 | 125.44 | 113.40 |
| 12 | f | 46 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 67 | 5 | 1357 | C | N3-C2-O2 | -5.47 | 118.07 | 121.90 |
| 67 | 5 | 2603 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 28 | ii | 290 | TYR | CB-CG-CD1 | -5.47 | 117.72 | 121.00 |
| 67 | 5 | 1626 | G | N3-C4-N9 | -5.47 | 122.72 | 126.00 |
| 67 | 5 | 1857 | C | C5-C4-N4 | -5.47 | 116.37 | 120.20 |
| 67 | 5 | 1938 | C | C6-N1-C1' | -5.47 | 114.24 | 120.80 |
| 67 | 5 | 2871 | A | N1-C6-N6 | 5.47 | 121.88 | 118.60 |
| 67 | 5 | 3612 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 67 | 5 | 339 | C | C6-N1-C1' | -5.47 | 114.24 | 120.80 |
| 67 | 5 | 5004 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 67 | 5 | 3909 | C | C5-C4-N4 | -5.47 | 116.37 | 120.20 |
| 67 | 5 | 4333 | C | C5-C4-N4 | -5.47 | 116.37 | 120.20 |
| 67 | 5 | 4868 | G | C8-N9-C1' | -5.47 | 119.89 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 418 | A | C4-N9-C1' | 5.46 | 136.13 | 126.30 |
| 67 | 5 | 1803 | G | C8-N9-C4 | 5.46 | 108.58 | 106.40 |
| 67 | 5 | 2739 | C | N3-C4-C5 | 5.46 | 124.08 | 121.90 |
| 67 | 5 | 4213 | A | C8-N9-C4 | -5.46 | 103.61 | 105.80 |
| 67 | 5 | 3857 | G | N3-C4-C5 | -5.46 | 125.87 | 128.60 |
| 67 | 5 | 4598 | C | C5-C4-N4 | -5.46 | 116.38 | 120.20 |
| 76 | 9 | 672 | A | N1-C6-N6 | 5.46 | 121.88 | 118.60 |
| 67 | 5 | 651 | C | C6-N1-C1' | -5.46 | 114.25 | 120.80 |
| 67 | 5 | 4335 | C | N3-C4-C5 | 5.46 | 124.08 | 121.90 |
| 76 | 9 | 1490 | G | C8-N9-C1' | -5.46 | 119.90 | 127.00 |
| 67 | 5 | 1777 | C | C2-N1-C1' | 5.46 | 124.80 | 118.80 |
| 67 | 5 | 1945 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 67 | 5 | 4513 | A | C6-N1-C2 | -5.46 | 115.33 | 118.60 |
| 70 | 7 | 97 | G | N3-C2-N2 | -5.46 | 116.08 | 119.90 |
| 67 | 5 | 229 | G | C4-C5-N7 | 5.46 | 112.98 | 110.80 |
| 67 | 5 | 2001 | G | C8-N9-C1' | 5.46 | 134.09 | 127.00 |
| 67 | 5 | 80 | C | N3-C2-O2 | -5.45 | 118.08 | 121.90 |
| 73 | 8 | 150 | C | N3-C4-N4 | -5.45 | 114.18 | 118.00 |
| 76 | 9 | 215 | G | N3-C4-C5 | 5.45 | 131.33 | 128.60 |
| 76 | 9 | 1760 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 76 | 9 | 1245 | G | C2-N3-C4 | 5.45 | 114.63 | 111.90 |
| 32 | jj | 569 | LEU | CA-CB-CG | 5.45 | 127.84 | 115.30 |
| 76 | 9 | 1226 | G | N7-C8-N9 | 5.45 | 115.83 | 113.10 |
| 76 | 9 | 1230 | C | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 67 | 5 | 39 | A | C4-C5-C6 | 5.45 | 119.72 | 117.00 |
| 67 | 5 | 2622 | G | C8-N9-C1' | -5.45 | 119.92 | 127.00 |
| 67 | 5 | 3760 | A | C5-C6-N6 | 5.45 | 128.06 | 123.70 |
| 67 | 5 | 3840 | U | O4'-C1'-N1 | 5.45 | 112.56 | 108.20 |
| 67 | 5 | 1941 | A | C5-C6-N6 | 5.45 | 128.06 | 123.70 |
| 67 | 5 | 2381 | A | C5-C6-N6 | 5.45 | 128.06 | 123.70 |
| 67 | 5 | 3696 | C | C2-N1-C1' | 5.45 | 124.79 | 118.80 |
| 76 | 9 | 545 | A | N1-C6-N6 | 5.45 | 121.87 | 118.60 |
| 82 | c | 42 | LYS | CD-CE-NZ | 5.44 | 124.22 | 111.70 |
| 4 | DD | 76 | ARG | NE-CZ-NH1 | 5.44 | 123.02 | 120.30 |
| 32 | jj | 379 | LEU | CB-CG-CD2 | -5.44 | 101.75 | 111.00 |
| 67 | 5 | 39 | A | N7-C8-N9 | 5.44 | 116.52 | 113.80 |
| 67 | 5 | 199 | G | O4'-C1'-N9 | 5.44 | 112.55 | 108.20 |
| 67 | 5 | 2435 | G | C2-N3-C4 | -5.44 | 109.18 | 111.90 |
| 67 | 5 | 4277 | G | N3-C4-N9 | 5.44 | 129.27 | 126.00 |
| 67 | 5 | 4668 | U | O5'-P-OP1 | -5.44 | 100.80 | 105.70 |
| 67 | 5 | 4701 | A | C8-N9-C1' | 5.44 | 137.50 | 127.70 |
| 73 | 8 | 8 | U | C2-N1-C1' | 5.44 | 124.23 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | 9 | 1294 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 67 | 5 | 39 | A | C6-C5-N7 | -5.44 | 128.49 | 132.30 |
| 67 | 5 | 1884 | C | N1-C2-O2 | 5.44 | 122.16 | 118.90 |
| 70 | 7 | 36 | C | C6-N1-C1' | -5.44 | 114.27 | 120.80 |
| 67 | 5 | 4204 | C | C2-N1-C1' | 5.44 | 124.78 | 118.80 |
| 67 | 5 | 111 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 67 | 5 | 283 | G | C8-N9-C1' | -5.44 | 119.93 | 127.00 |
| 67 | 5 | 749 | G | C2-N3-C4 | -5.44 | 109.18 | 111.90 |
| 67 | 5 | 2006 | U | O4'-C1'-N1 | 5.44 | 112.55 | 108.20 |
| 67 | 5 | 2815 | A | C4-N9-C1' | 5.44 | 136.09 | 126.30 |
| 76 | 9 | 123 | G | N3-C4-C5 | -5.44 | 125.88 | 128.60 |
| 76 | 9 | 1849 | G | C6-C5-N7 | -5.44 | 127.14 | 130.40 |
| 67 | 5 | 1811 | G | N3-C4-N9 | -5.43 | 122.74 | 126.00 |
| 67 | 5 | 4088 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 67 | 5 | 4579 | U | N3-C4-O4 | 5.43 | 123.20 | 119.40 |
| 76 | 9 | 1638 | G | C8-N9-C1' | 5.43 | 134.06 | 127.00 |
| 67 | 5 | 3835 | C | C2-N1-C1' | 5.43 | 124.78 | 118.80 |
| 67 | 5 | 4604 | G | C8-N9-C1' | -5.43 | 119.94 | 127.00 |
| 67 | 5 | 1629 | G | N1-C6-O6 | 5.43 | 123.16 | 119.90 |
| 67 | 5 | 1573 | G | C8-N9-C4 | -5.43 | 104.23 | 106.40 |
| 67 | 5 | 2276 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 67 | 5 | 3630 | A | N1-C6-N6 | -5.43 | 115.34 | 118.60 |
| 67 | 5 | 4412 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |
| 70 | 7 | 15 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |
| 76 | 9 | 1527 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 76 | 9 | 1860 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 67 | 5 | 962 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 67 | 5 | 3617 | G | N3-C4-N9 | -5.43 | 122.74 | 126.00 |
| 67 | 5 | 4374 | U | O4'-C1'-N1 | -5.43 | 103.86 | 108.20 |
| 67 | 5 | 1216 | C | C6-N1-C2 | 5.42 | 122.47 | 120.30 |
| 67 | 5 | 4511 | A | N1-C6-N6 | -5.42 | 115.35 | 118.60 |
| 8 | EE | 162 | ILE | CG1-CB-CG2 | -5.42 | 99.47 | 111.40 |
| 67 | 5 | 2895 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 67 | 5 | 3692 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 73 | 8 | 96 | C | N3-C4-N4 | 5.42 | 121.80 | 118.00 |
| 73 | 8 | 121 | G | C2-N3-C4 | -5.42 | 109.19 | 111.90 |
| 67 | 5 | 1553 | A | N1-C6-N6 | 5.42 | 121.85 | 118.60 |
| 67 | 5 | 1883 | G | O4'-C1'-N9 | -5.42 | 103.86 | 108.20 |
| 67 | 5 | 2429 | A | C6-N1-C2 | -5.42 | 115.35 | 118.60 |
| 67 | 5 | 4179 | G | N3-C2-N2 | 5.42 | 123.69 | 119.90 |
| 76 | 9 | 1274 | G | N3-C2-N2 | 5.42 | 123.69 | 119.90 |
| 67 | 5 | 4726 | G | C2-N3-C4 | -5.42 | 109.19 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4169 | G | N1-C2-N2 | -5.42 | 111.32 | 116.20 |
| 67 | 5 | 4517 | A | C6-N1-C2 | -5.42 | 115.35 | 118.60 |
| 67 | 5 | 4945 | G | N9-C4-C5 | -5.42 | 103.23 | 105.40 |
| 76 | 9 | 587 | A | O4'-C1'-N9 | -5.42 | 103.86 | 108.20 |
| 67 | 5 | 315 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 67 | 5 | 713 | C | N1-C2-O2 | 5.42 | 122.15 | 118.90 |
| 67 | 5 | 2860 | C | C2-N1-C1' | 5.42 | 124.76 | 118.80 |
| 76 | 9 | 1327 | G | C4-N9-C1' | 5.42 | 133.54 | 126.50 |
| 67 | 5 | 89 | C | N3-C2-O2 | -5.42 | 118.11 | 121.90 |
| 67 | 5 | 4744 | A | O4'-C1'-N9 | -5.42 | 103.87 | 108.20 |
| 67 | 5 | 210 | C | N3-C4-C5 | 5.41 | 124.07 | 121.90 |
| 67 | 5 | 2379 | A | C4-N9-C1' | 5.41 | 136.04 | 126.30 |
| 67 | 5 | 4239 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 73 | 8 | 41 | A | N1-C6-N6 | -5.41 | 115.35 | 118.60 |
| 73 | 8 | 148 | A | C5-C6-N1 | 5.41 | 120.41 | 117.70 |
| 67 | 5 | 1803 | G | N9-C4-C5 | -5.41 | 103.23 | 105.40 |
| 67 | 5 | 1549 | G | C8-N9-C4 | -5.41 | 104.24 | 106.40 |
| 67 | 5 | 1584 | G | N1-C6-O6 | 5.41 | 123.15 | 119.90 |
| 67 | 5 | 4087 | G | C4-N9-C1' | -5.41 | 119.47 | 126.50 |
| 67 | 5 | 4330 | G | N3-C4-C5 | -5.41 | 125.89 | 128.60 |
| 67 | 5 | 352 | G | C2-N3-C4 | -5.41 | 109.19 | 111.90 |
| 67 | 5 | 1788 | A | O4'-C1'-N9 | 5.41 | 112.53 | 108.20 |
| 67 | 5 | 1842 | G | N3-C2-N2 | 5.41 | 123.69 | 119.90 |
| 67 | 5 | 4550 | G | N1-C2-N3 | 5.41 | 127.14 | 123.90 |
| 67 | 5 | 55 | G | N3-C4-C5 | -5.41 | 125.90 | 128.60 |
| 76 | 9 | 669 | A | C8-N9-C1' | -5.41 | 117.97 | 127.70 |
| 67 | 5 | 1310 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 67 | 5 | 2871 | A | C5-C6-N6 | -5.41 | 119.38 | 123.70 |
| 70 | 7 | 109 | U | C2-N1-C1' | 5.41 | 124.19 | 117.70 |
| 73 | 8 | 26 | C | C6-N1-C1' | -5.41 | 114.31 | 120.80 |
| 67 | 5 | 4394 | A | C5-C6-N6 | -5.40 | 119.38 | 123.70 |
| 67 | 5 | 1651 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 67 | 5 | 1626 | G | N3-C4-C5 | 5.40 | 131.30 | 128.60 |
| 76 | 9 | 1394 | G | O4'-C1'-N9 | -5.40 | 103.88 | 108.20 |
| 67 | 5 | 2478 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 67 | 5 | 2691 | U | C6-N1-C2 | -5.40 | 117.76 | 121.00 |
| 67 | 5 | 4092 | G | C4-N9-C1' | 5.40 | 133.52 | 126.50 |
| 67 | 5 | 4978 | G | N1-C2-N2 | -5.40 | 111.34 | 116.20 |
| 67 | 5 | 1589 | C | N3-C2-O2 | -5.40 | 118.12 | 121.90 |
| 67 | 5 | 2591 | A | N1-C6-N6 | 5.40 | 121.84 | 118.60 |
| 76 | 9 | 1280 | G | N3-C4-N9 | 5.40 | 129.24 | 126.00 |
| 76 | 9 | 1413 | G | C8-N9-C1' | -5.40 | 119.98 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1577 | G | C4-N9-C1' | 5.39 | 133.51 | 126.50 |
| 67 | 5 | 4522 | G | C4-C5-N7 | 5.39 | 112.96 | 110.80 |
| 76 | 9 | 1666 | C | C6-N1-C1' | -5.39 | 114.33 | 120.80 |
| 76 | 9 | 1588 | A | C5-C6-N6 | 5.39 | 128.01 | 123.70 |
| 67 | 5 | 1510 | G | C4-N9-C1' | 5.39 | 133.51 | 126.50 |
| 67 | 5 | 1893 | C | O4'-C1'-N1 | 5.39 | 112.51 | 108.20 |
| 67 | 5 | 3783 | A | O4'-C1'-N9 | 5.39 | 112.51 | 108.20 |
| 76 | 9 | 391 | C | C2-N1-C1' | 5.39 | 124.73 | 118.80 |
| 67 | 5 | 401 | G | N3-C4-C5 | -5.39 | 125.91 | 128.60 |
| 67 | 5 | 1346 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 67 | 5 | 3903 | A | C5-N7-C8 | -5.39 | 101.21 | 103.90 |
| 67 | 5 | 4623 | G | N7-C8-N9 | 5.39 | 115.79 | 113.10 |
| 67 | 5 | 2615 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 67 | 5 | 75 | G | N1-C2-N2 | -5.38 | 111.35 | 116.20 |
| 67 | 5 | 3857 | G | N3-C4-N9 | 5.38 | 129.23 | 126.00 |
| 67 | 5 | 2321 | G | N3-C4-C5 | 5.38 | 131.29 | 128.60 |
| 67 | 5 | 2509 | C | N1-C2-O2 | 5.38 | 122.13 | 118.90 |
| 67 | 5 | 3705 | G | C4-N9-C1' | 5.38 | 133.50 | 126.50 |
| 76 | 9 | 435 | A | N1-C6-N6 | -5.38 | 115.37 | 118.60 |
| 76 | 9 | 886 | A | N1-C6-N6 | -5.38 | 115.37 | 118.60 |
| 67 | 5 | 1594 | C | N3-C4-C5 | 5.38 | 124.05 | 121.90 |
| 67 | 5 | 1668 | A | N1-C6-N6 | -5.38 | 115.37 | 118.60 |
| 67 | 5 | 1552 | G | C2-N3-C4 | -5.38 | 109.21 | 111.90 |
| 67 | 5 | 1573 | G | N9-C1'-C2' | 5.38 | 120.99 | 114.00 |
| 67 | 5 | 643 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 67 | 5 | 2033 | A | C5-C6-N6 | -5.38 | 119.40 | 123.70 |
| 67 | 5 | 4978 | G | C8-N9-C1' | -5.38 | 120.01 | 127.00 |
| 67 | 5 | 4688 | C | C6-N1-C1' | -5.38 | 114.35 | 120.80 |
| 73 | 8 | 150 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 76 | 9 | 1798 | C | N3-C2-O2 | -5.38 | 118.14 | 121.90 |
| 67 | 5 | 3752 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 67 | 5 | 1308 | C | C6-N1-C1' | -5.37 | 114.35 | 120.80 |
| 67 | 5 | 1310 | C | C2-N1-C1' | 5.37 | 124.71 | 118.80 |
| 67 | 5 | 4701 | A | N1-C6-N6 | -5.37 | 115.38 | 118.60 |
| 67 | 5 | 2539 | C | C2-N1-C1' | 5.37 | 124.71 | 118.80 |
| 67 | 5 | 2640 | G | C4-N9-C1' | 5.37 | 133.48 | 126.50 |
| 67 | 5 | 2847 | G | C8-N9-C4 | -5.37 | 104.25 | 106.40 |
| 67 | 5 | 732 | A | C5-C6-N6 | -5.37 | 119.41 | 123.70 |
| 69 | X | 147 | LEU | CB-CG-CD2 | -5.37 | 101.87 | 111.00 |
| 76 | 9 | 1425 | G | C8-N9-C1' | -5.37 | 120.02 | 127.00 |
| 67 | 5 | 2544 | G | C8-N9-C1' | -5.37 | 120.02 | 127.00 |
| 67 | 5 | 2654 | C | C2-N1-C1' | 5.37 | 124.70 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 70 | 7 | 29 | C | N3-C4-C5 | 5.37 | 124.05 | 121.90 |
| 67 | 5 | 1411(C) | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 67 | 5 | 4317 | A | C6-N1-C2 | -5.37 | 115.38 | 118.60 |
| 76 | 9 | 52 | G | C8-N9-C4 | 5.37 | 108.55 | 106.40 |
| 76 | 9 | 1335 | G | N3-C2-N2 | 5.37 | 123.66 | 119.90 |
| 76 | 9 | 1664 | A | N1-C6-N6 | -5.37 | 115.38 | 118.60 |
| 67 | 5 | 917 | A | N1-C6-N6 | 5.36 | 121.82 | 118.60 |
| 67 | 5 | 1529 | G | N7-C8-N9 | 5.36 | 115.78 | 113.10 |
| 67 | 5 | 3882 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |
| 67 | 5 | 2670 | C | C5-C4-N4 | -5.36 | 116.45 | 120.20 |
| 76 | 9 | 1563 | G | N9-C4-C5 | -5.36 | 103.26 | 105.40 |
| 67 | 5 | 221 | C | C6-N1-C1' | -5.36 | 114.37 | 120.80 |
| 76 | 9 | 390 | C | C6-N1-C1' | -5.36 | 114.37 | 120.80 |
| 32 | jj | 292 | PHE | CB-CG-CD1 | 5.36 | 124.55 | 120.80 |
| 67 | 5 | 1619 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 67 | 5 | 1803 | G | C2-N3-C4 | -5.36 | 109.22 | 111.90 |
| 67 | 5 | 2438 | A | C5-C6-N6 | -5.36 | 119.42 | 123.70 |
| 67 | 5 | 2621 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 67 | 5 | 3654 | G | C2-N3-C4 | -5.36 | 109.22 | 111.90 |
| 67 | 5 | 666 | G | C4-N9-C1' | -5.36 | 119.54 | 126.50 |
| 67 | 5 | 1577 | G | C8-N9-C1' | -5.36 | 120.04 | 127.00 |
| 67 | 5 | 52 | G | C8-N9-C1' | -5.35 | 120.04 | 127.00 |
| 67 | 5 | 343 | C | C2-N1-C1' | 5.35 | 124.69 | 118.80 |
| 67 | 5 | 1282 | G | C6-C5-N7 | -5.35 | 127.19 | 130.40 |
| 67 | 5 | 3665 | G | C8-N9-C1' | -5.35 | 120.04 | 127.00 |
| 67 | 5 | 33 | A | C5-N7-C8 | -5.35 | 101.22 | 103.90 |
| 67 | 5 | 51 | A | N9-C4-C5 | -5.35 | 103.66 | 105.80 |
| 67 | 5 | 66 | A | C8-N9-C4 | -5.35 | 103.66 | 105.80 |
| 67 | 5 | 135 | G | N3-C2-N2 | 5.35 | 123.64 | 119.90 |
| 67 | 5 | 3813 | A | C8-N9-C1' | -5.35 | 118.07 | 127.70 |
| 67 | 5 | 4603 | C | C6-N1-C1' | -5.35 | 114.38 | 120.80 |
| 76 | 9 | 1014 | G | C6-C5-N7 | -5.35 | 127.19 | 130.40 |
| 67 | 5 | 320 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 73 | 8 | 47 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 76 | 9 | 1019 | C | C5-C6-N1 | 5.35 | 123.67 | 121.00 |
| 67 | 5 | 1655 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 67 | 5 | 1794 | A | N1-C6-N6 | 5.34 | 121.81 | 118.60 |
| 67 | 5 | 2603 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 67 | 5 | 4522 | G | N3-C2-N2 | 5.34 | 123.64 | 119.90 |
| 67 | 5 | 1690 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 67 | 5 | 3857 | G | C8-N9-C4 | -5.34 | 104.26 | 106.40 |
| 67 | 5 | 707 | C | C2-N1-C1' | 5.34 | 124.68 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2824 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 67 | 5 | 3894 | A | C8-N9-C1' | -5.34 | 118.09 | 127.70 |
| 67 | 5 | 4485 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 76 | 9 | 1474 | A | N1-C6-N6 | -5.34 | 115.40 | 118.60 |
| 76 | 9 | 1702 | G | N1-C6-O6 | -5.34 | 116.69 | 119.90 |
| 43 | n | 18 | ARG | CG-CD-NE | 5.34 | 123.01 | 111.80 |
| 67 | 5 | 356 | G | C4-N9-C1' | 5.34 | 133.44 | 126.50 |
| 67 | 5 | 414 | C | O4'-C1'-N1 | 5.34 | 112.47 | 108.20 |
| 67 | 5 | 1541 | C | N3-C4-N4 | 5.34 | 121.74 | 118.00 |
| 67 | 5 | 2737 | C | C5-C4-N4 | -5.34 | 116.46 | 120.20 |
| 63 | UU | 39 | LEU | CA-CB-CG | -5.34 | 103.03 | 115.30 |
| 67 | 5 | 90 | G | C8-N9-C1' | -5.34 | 120.06 | 127.00 |
| 67 | 5 | 4565 | C | C6-N1-C2 | -5.34 | 118.17 | 120.30 |
| 67 | 5 | 1875 | C | C5-C4-N4 | -5.33 | 116.47 | 120.20 |
| 67 | 5 | 2863 | G | N1-C2-N3 | 5.33 | 127.10 | 123.90 |
| 67 | 5 | 686 | A | C5-C6-N6 | -5.33 | 119.43 | 123.70 |
| 67 | 5 | 2318 | G | N3-C2-N2 | 5.33 | 123.63 | 119.90 |
| 67 | 5 | 2468 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 67 | 5 | 2518 | G | C2-N3-C4 | -5.33 | 109.23 | 111.90 |
| 73 | 8 | 19 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 67 | 5 | 1842 | G | N1-C2-N2 | -5.33 | 111.40 | 116.20 |
| 67 | 5 | 1729 | A | C6-N1-C2 | -5.33 | 115.40 | 118.60 |
| 76 | 9 | 1079 | C | C5-C4-N4 | -5.33 | 116.47 | 120.20 |
| 67 | 5 | 4194 | U | C5-C4-O4 | 5.33 | 129.10 | 125.90 |
| 73 | 8 | 141 | C | C6-N1-C2 | -5.33 | 118.17 | 120.30 |
| 67 | 5 | 1081 | C | C2-N3-C4 | 5.33 | 122.56 | 119.90 |
| 67 | 5 | 3850 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 67 | 5 | 4388 | A | C6-N1-C2 | -5.33 | 115.40 | 118.60 |
| 50 | PP | 60 | LEU | CB-CG-CD2 | 5.32 | 120.05 | 111.00 |
| 67 | 5 | 228 | C | N3-C2-O2 | -5.32 | 118.17 | 121.90 |
| 67 | 5 | 4541 | G | C2-N3-C4 | -5.32 | 109.24 | 111.90 |
| 67 | 5 | 4645 | C | C6-N1-C1' | -5.32 | 114.41 | 120.80 |
| 67 | 5 | 2359 | U | P-O3'-C3' | 5.32 | 126.08 | 119.70 |
| 67 | 5 | 4305 | G | C5-N7-C8 | -5.32 | 101.64 | 104.30 |
| 76 | 9 | 884 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 45 | O | 52 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 67 | 5 | 2748 | C | C2-N3-C4 | -5.32 | 117.24 | 119.90 |
| 67 | 5 | 3867 | A | N9-C4-C5 | -5.32 | 103.67 | 105.80 |
| 67 | 5 | 221 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 67 | 5 | 285 | G | N1-C2-N3 | 5.32 | 127.09 | 123.90 |
| 67 | 5 | 1561 | G | C8-N9-C1' | -5.32 | 120.09 | 127.00 |
| 67 | 5 | 2748 | C | N3-C4-C5 | 5.32 | 124.03 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4087 | G | C2-N3-C4 | -5.32 | 109.24 | 111.90 |
| 67 | 5 | 1641 | G | N3-C4-N9 | -5.32 | 122.81 | 126.00 |
| 67 | 5 | 2493 | G | C4-N9-C1' | 5.32 | 133.41 | 126.50 |
| 67 | 5 | 4256 | A | C5-C6-N6 | -5.32 | 119.45 | 123.70 |
| 2 | C | 100 | ARG | CG-CD-NE | 5.31 | 122.96 | 111.80 |
| 67 | 5 | 1836 | G | C8-N9-C1' | -5.31 | 120.09 | 127.00 |
| 67 | 5 | 4553 | A | C8-N9-C1' | -5.31 | 118.14 | 127.70 |
| 76 | 9 | 1659 | U | C6-N1-C2 | -5.31 | 117.81 | 121.00 |
| 67 | 5 | 106 | A | N9-C4-C5 | -5.31 | 103.68 | 105.80 |
| 67 | 5 | 1830 | G | C8-N9-C1' | -5.31 | 120.10 | 127.00 |
| 67 | 5 | 1846 | G | N3-C4-C5 | -5.31 | 125.94 | 128.60 |
| 67 | 5 | 1998 | A | N1-C6-N6 | 5.31 | 121.79 | 118.60 |
| 67 | 5 | 2792 | C | N3-C2-O2 | -5.31 | 118.18 | 121.90 |
| 67 | 5 | 4298 | A | C5-C6-N1 | 5.31 | 120.36 | 117.70 |
| 67 | 5 | 2276 | A | C6-N1-C2 | -5.31 | 115.42 | 118.60 |
| 76 | 9 | 1327 | G | C8-N9-C1' | -5.31 | 120.10 | 127.00 |
| 76 | 9 | 925 | G | N3-C4-N9 | -5.31 | 122.82 | 126.00 |
| 76 | 9 | 1294 | G | N1-C2-N2 | -5.31 | 111.42 | 116.20 |
| 67 | 5 | 131 | C | C2-N1-C1' | 5.30 | 124.64 | 118.80 |
| 67 | 5 | 1610 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 67 | 5 | 2693 | G | N1-C2-N2 | -5.30 | 111.43 | 116.20 |
| 67 | 5 | 2607 | C | C2-N1-C1' | 5.30 | 124.63 | 118.80 |
| 55 | s | 6 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 67 | 5 | 1279 | A | N1-C6-N6 | 5.30 | 121.78 | 118.60 |
| 73 | 8 | 148 | A | C5-C6-N6 | -5.30 | 119.46 | 123.70 |
| 58 | t | 15 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 67 | 5 | 1789 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 76 | 9 | 897 | U | O4'-C1'-N1 | 5.30 | 112.44 | 108.20 |
| 76 | 9 | 1395 | C | C5'-C4'-O4' | 5.30 | 115.46 | 109.10 |
| 67 | 5 | 1546 | C | C5-C4-N4 | -5.30 | 116.49 | 120.20 |
| 67 | 5 | 3665 | G | C2-N3-C4 | -5.30 | 109.25 | 111.90 |
| 67 | 5 | 4214 | A | C6-N1-C2 | -5.30 | 115.42 | 118.60 |
| 67 | 5 | 241 | G | C4-N9-C1' | 5.30 | 133.38 | 126.50 |
| 67 | 5 | 2379 | A | N1-C6-N6 | 5.30 | 121.78 | 118.60 |
| 67 | 5 | 4581 | G | C2-N3-C4 | -5.30 | 109.25 | 111.90 |
| 67 | 5 | 2050 | G | C6-C5-N7 | -5.29 | 127.22 | 130.40 |
| 67 | 5 | 2093 | G | P-O3'-C3' | 5.29 | 126.05 | 119.70 |
| 67 | 5 | 2404 | A | C5-C6-N1 | 5.29 | 120.35 | 117.70 |
| 76 | 9 | 1314 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 67 | 5 | 240 | G | C8-N9-C1' | -5.29 | 120.12 | 127.00 |
| 67 | 5 | 3649 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 76 | 9 | 1515 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 148 | A | N9-C4-C5 | -5.29 | 103.68 | 105.80 |
| 76 | 9 | 677 | G | C4-N9-C1' | 5.29 | 133.38 | 126.50 |
| 76 | 9 | 1394 | G | C4-N9-C1' | 5.29 | 133.38 | 126.50 |
| 67 | 5 | 1869 | G | C4-N9-C1' | 5.29 | 133.38 | 126.50 |
| 67 | 5 | 4622 | A | C5-C6-N1 | 5.29 | 120.34 | 117.70 |
| 76 | 9 | 480 | G | C6-C5-N7 | -5.29 | 127.23 | 130.40 |
| 67 | 5 | 2664 | G | N3-C4-N9 | -5.29 | 122.83 | 126.00 |
| 67 | 5 | 53 | C | N1-C2-O2 | 5.29 | 122.07 | 118.90 |
| 67 | 5 | 3649 | A | C5-C6-N1 | 5.29 | 120.34 | 117.70 |
| 67 | 5 | 3916 | G | C4-N9-C1' | 5.29 | 133.37 | 126.50 |
| 67 | 5 | 3841 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 67 | 5 | 4723 | A | N3-C4-C5 | -5.28 | 123.10 | 126.80 |
| 70 | 7 | 115 | A | C5-C6-N1 | 5.28 | 120.34 | 117.70 |
| 67 | 5 | 409 | G | N7-C8-N9 | 5.28 | 115.74 | 113.10 |
| 67 | 5 | 969 | C | N3-C2-O2 | -5.28 | 118.20 | 121.90 |
| 67 | 5 | 2603 | C | C6-N1-C1' | -5.28 | 114.47 | 120.80 |
| 67 | 5 | 2772 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 20 | G | 199 | LEU | CB-CG-CD2 | -5.28 | 102.03 | 111.00 |
| 67 | 5 | 4902 | C | C6-N1-C1' | -5.28 | 114.47 | 120.80 |
| 67 | 5 | 4487 | A | N1-C6-N6 | 5.28 | 121.77 | 118.60 |
| 67 | 5 | 4604 | G | C4-N9-C1' | 5.28 | 133.36 | 126.50 |
| 67 | 5 | 4920 | C | N1-C1'-C2' | -5.28 | 106.20 | 112.00 |
| 76 | 9 | 1389 | C | N1-C2-O2 | 5.28 | 122.06 | 118.90 |
| 76 | 9 | 1715 | A | N9-C4-C5 | -5.28 | 103.69 | 105.80 |
| 76 | 9 | 656 | G | C4-N9-C1' | 5.27 | 133.36 | 126.50 |
| 67 | 5 | 1065 | G | N1-C6-O6 | -5.27 | 116.74 | 119.90 |
| 67 | 5 | 1316 | G | C8-N9-C1' | -5.27 | 120.14 | 127.00 |
| 67 | 5 | 2010 | A | O4'-C1'-N9 | 5.27 | 112.42 | 108.20 |
| 67 | 5 | 2848 | G | C5-C6-N1 | -5.27 | 108.86 | 111.50 |
| 76 | 9 | 11 | A | N9-C4-C5 | -5.27 | 103.69 | 105.80 |
| 76 | 9 | 1603 | G | N3-C2-N2 | 5.27 | 123.59 | 119.90 |
| 67 | 5 | 2807 | A | C5-C6-N1 | 5.27 | 120.34 | 117.70 |
| 76 | 9 | 611 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 11 | E | 208 | GLY | N-CA-C | 5.27 | 126.28 | 113.10 |
| 67 | 5 | 1277 | G | C2-N3-C4 | -5.27 | 109.27 | 111.90 |
| 67 | 5 | 3807 | A | C5-C6-N1 | 5.27 | 120.33 | 117.70 |
| 67 | 5 | 4183 | G | N3-C4-N9 | -5.27 | 122.84 | 126.00 |
| 73 | 8 | 87 | G | C2-N3-C4 | -5.27 | 109.27 | 111.90 |
| 76 | 9 | 1740 | C | N3-C4-N4 | 5.27 | 121.69 | 118.00 |
| 67 | 5 | 344 | A | C6-N1-C2 | -5.27 | 115.44 | 118.60 |
| 67 | 5 | 1651 | G | C2-N3-C4 | -5.27 | 109.27 | 111.90 |
| 67 | 5 | 1929 | A | C6-N1-C2 | -5.27 | 115.44 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4370 | G | C8-N9-C1' | -5.27 | 120.15 | 127.00 |
| 67 | 5 | 4506 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 76 | 9 | 1757 | G | C4-N9-C1' | 5.27 | 133.35 | 126.50 |
| 67 | 5 | 301 | G | N1-C2-N3 | 5.27 | 127.06 | 123.90 |
| 67 | 5 | 1561 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 76 | 9 | 1454 | A | C5-C6-N6 | 5.27 | 127.91 | 123.70 |
| 76 | 9 | 1619 | A | C5-C6-N6 | -5.27 | 119.49 | 123.70 |
| 67 | 5 | 434 | A | C5-C6-N6 | -5.26 | 119.49 | 123.70 |
| 67 | 5 | 1300 | G | N3-C4-C5 | 5.26 | 131.23 | 128.60 |
| 67 | 5 | 2726 | G | C4-C5-N7 | 5.26 | 112.91 | 110.80 |
| 67 | 5 | 3945 | A | O3'-P-O5' | 5.26 | 114.00 | 104.00 |
| 76 | 9 | 1699 | A | N9-C4-C5 | -5.26 | 103.69 | 105.80 |
| 73 | 8 | 50 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 76 | 9 | 1147 | C | C5-C4-N4 | -5.26 | 116.52 | 120.20 |
| 76 | 9 | 1330 | G | N3-C4-N9 | -5.26 | 122.84 | 126.00 |
| 73 | 8 | 141 | C | C2-N1-C1' | 5.26 | 124.59 | 118.80 |
| 76 | 9 | 853 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 67 | 5 | 2259 | G | C8-N9-C1' | -5.26 | 120.16 | 127.00 |
| 67 | 5 | 2850 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |
| 67 | 5 | 4578 | G | C4-N9-C1' | 5.26 | 133.34 | 126.50 |
| 67 | 5 | 4695 | C | C6-N1-C2 | 5.26 | 122.40 | 120.30 |
| 76 | 9 | 18 | C | N3-C4-N4 | 5.26 | 121.68 | 118.00 |
| 67 | 5 | 2403 | A | C8-N9-C4 | -5.26 | 103.70 | 105.80 |
| 67 | 5 | 3691 | G | N1-C2-N3 | 5.26 | 127.06 | 123.90 |
| 76 | 9 | 1513 | C | C5-C4-N4 | 5.26 | 123.88 | 120.20 |
| 81 | B | 17 | LEU | CB-CG-CD2 | -5.26 | 102.06 | 111.00 |
| 62 | U | 19 | LEU | CB-CG-CD2 | 5.26 | 119.94 | 111.00 |
| 67 | 5 | 344 | A | C5-C6-N1 | 5.26 | 120.33 | 117.70 |
| 67 | 5 | 353 | A | N9-C4-C5 | -5.26 | 103.70 | 105.80 |
| 67 | 5 | 4179 | G | C6-C5-N7 | -5.26 | 127.25 | 130.40 |
| 67 | 5 | 106 | A | C5-N7-C8 | -5.25 | 101.27 | 103.90 |
| 67 | 5 | 2840 | A | C6-N1-C2 | -5.25 | 115.45 | 118.60 |
| 67 | 5 | 1329 | G | N7-C8-N9 | 5.25 | 115.73 | 113.10 |
| 67 | 5 | 1383 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |
| 67 | 5 | 1857 | C | N3-C4-C5 | 5.25 | 124.00 | 121.90 |
| 67 | 5 | 1916 | G | N1-C2-N2 | -5.25 | 111.47 | 116.20 |
| 67 | 5 | 2289 | C | C5-C4-N4 | -5.25 | 116.52 | 120.20 |
| 76 | 9 | 291 | G | C4-N9-C1' | 5.25 | 133.33 | 126.50 |
| 67 | 5 | 2737 | C | C2-N1-C1' | 5.25 | 124.58 | 118.80 |
| 76 | 9 | 1858 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 67 | 5 | 384 | A | C5-C6-N6 | 5.25 | 127.90 | 123.70 |
| 67 | 5 | 1910 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4462 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 76 | 9 | 1055 | A | C8-N9-C1' | -5.25 | 118.25 | 127.70 |
| 67 | 5 | 2583 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 67 | 5 | 4991 | U | C2-N1-C1' | 5.25 | 124.00 | 117.70 |
| 76 | 9 | 876 | C | C6-N1-C1' | -5.25 | 114.50 | 120.80 |
| 76 | 9 | 1459 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 67 | 5 | 666 | G | N1-C2-N2 | 5.25 | 120.92 | 116.20 |
| 67 | 5 | 4553 | A | C4-N9-C1' | 5.25 | 135.74 | 126.30 |
| 76 | 9 | 71 | G | C8-N9-C1' | -5.25 | 120.18 | 127.00 |
| 67 | 5 | 4314 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 67 | 5 | 4327 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 67 | 5 | 4375 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 76 | 9 | 1354 | G | N1-C2-N2 | -5.24 | 111.48 | 116.20 |
| 67 | 5 | 289 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 67 | 5 | 362 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 67 | 5 | 1298 | C | C2-N1-C1' | 5.24 | 124.56 | 118.80 |
| 67 | 5 | 2820 | C | C5-C4-N4 | -5.24 | 116.53 | 120.20 |
| 67 | 5 | 4945 | G | C4-C5-N7 | 5.24 | 112.90 | 110.80 |
| 67 | 5 | 15 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 67 | 5 | 756 | G | N3-C4-N9 | -5.24 | 122.86 | 126.00 |
| 67 | 5 | 1178 | G | C8-N9-C4 | -5.24 | 104.30 | 106.40 |
| 67 | 5 | 1887 | G | C2-N3-C4 | -5.24 | 109.28 | 111.90 |
| 67 | 5 | 4259 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 76 | 9 | 547 | G | C4-N9-C1' | 5.24 | 133.31 | 126.50 |
| 67 | 5 | 1326 | A | C8-N9-C4 | -5.24 | 103.71 | 105.80 |
| 67 | 5 | 1651 | G | C4-C5-N7 | 5.24 | 112.89 | 110.80 |
| 67 | 5 | 4669 | A | C8-N9-C4 | -5.24 | 103.71 | 105.80 |
| 67 | 5 | 4989 | U | C6-N1-C2 | -5.24 | 117.86 | 121.00 |
| 67 | 5 | 313 | U | C5-C4-O4 | -5.23 | 122.76 | 125.90 |
| 67 | 5 | 1908 | A | C5-C6-N6 | -5.23 | 119.51 | 123.70 |
| 67 | 5 | 1980 | U | P-O3'-C3' | -5.23 | 113.42 | 119.70 |
| 67 | 5 | 2075 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 67 | 5 | 3858 | C | C6-N1-C1' | -5.23 | 114.52 | 120.80 |
| 67 | 5 | 4868 | G | N3-C4-N9 | 5.23 | 129.14 | 126.00 |
| 70 | 7 | 93 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 76 | 9 | 1144 | A | C5-C6-N6 | -5.23 | 119.51 | 123.70 |
| 44 | NN | 124 | ARG | NE-CZ-NH2 | -5.23 | 117.69 | 120.30 |
| 67 | 5 | 1908 | A | C5-N7-C8 | -5.23 | 101.28 | 103.90 |
| 67 | 5 | 3744 | G | N1-C2-N2 | -5.23 | 111.49 | 116.20 |
| 67 | 5 | 4279 | A | C6-C5-N7 | -5.23 | 128.64 | 132.30 |
| 67 | 5 | 4448 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 67 | 5 | 4499 | G | C8-N9-C1' | -5.23 | 120.20 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 353 | A | C6-C5-N7 | -5.23 | 128.64 | 132.30 |
| 67 | 5 | 415 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 67 | 5 | 1658 | G | C4-N9-C1' | 5.23 | 133.29 | 126.50 |
| 67 | 5 | 4082 | G | N3-C4-C5 | -5.23 | 125.99 | 128.60 |
| 67 | 5 | 4091 | G | C4-N9-C1' | 5.23 | 133.30 | 126.50 |
| 67 | 5 | 4164 | C | N3-C2-O2 | -5.23 | 118.24 | 121.90 |
| 70 | 7 | 82 | G | C8-N9-C1' | -5.23 | 120.20 | 127.00 |
| 76 | 9 | 321 | C | C5-C4-N4 | -5.23 | 116.54 | 120.20 |
| 67 | 5 | 1321 | G | C8-N9-C1' | -5.23 | 120.21 | 127.00 |
| 76 | 9 | 1474 | A | C5-N7-C8 | 5.23 | 106.51 | 103.90 |
| 67 | 5 | 401 | G | N3-C4-N9 | 5.22 | 129.13 | 126.00 |
| 67 | 5 | 3671 | G | C2-N3-C4 | -5.22 | 109.29 | 111.90 |
| 76 | 9 | 1459 | G | C4-C5-N7 | 5.22 | 112.89 | 110.80 |
| 67 | 5 | 1846 | G | N1-C2-N2 | -5.22 | 111.50 | 116.20 |
| 67 | 5 | 1941 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 67 | 5 | 2690 | C | C6-N1-C1' | -5.22 | 114.53 | 120.80 |
| 67 | 5 | 2578 | G | C4-N9-C1' | 5.22 | 133.29 | 126.50 |
| 67 | 5 | 3909 | C | C5-C6-N1 | -5.22 | 118.39 | 121.00 |
| 67 | 5 | 19 | G | C8-N9-C1' | -5.22 | 120.21 | 127.00 |
| 67 | 5 | 1868 | A | C6-C5-N7 | -5.22 | 128.65 | 132.30 |
| 67 | 5 | 1877 | G | N3-C2-N2 | 5.22 | 123.55 | 119.90 |
| 67 | 5 | 1879 | C | N3-C2-O2 | -5.22 | 118.25 | 121.90 |
| 67 | 5 | 1938 | C | C2-N3-C4 | -5.21 | 117.29 | 119.90 |
| 67 | 5 | 2018 | C | P-O3'-C3' | 5.21 | 125.96 | 119.70 |
| 67 | 5 | 3813 | A | C4-N9-C1' | 5.21 | 135.69 | 126.30 |
| 67 | 5 | 4394 | A | C5-N7-C8 | -5.21 | 101.29 | 103.90 |
| 67 | 5 | 4454 | G | N3-C2-N2 | 5.21 | 123.55 | 119.90 |
| 76 | 9 | 810 | A | N9-C4-C5 | -5.21 | 103.71 | 105.80 |
| 76 | 9 | 1610 | G | C6-C5-N7 | -5.21 | 127.27 | 130.40 |
| 67 | 5 | 2343 | G | C8-N9-C1' | -5.21 | 120.22 | 127.00 |
| 67 | 5 | 3901 | A | N1-C6-N6 | 5.21 | 121.73 | 118.60 |
| 67 | 5 | 1898 | C | C6-N1-C2 | 5.21 | 122.38 | 120.30 |
| 76 | 9 | 1654 | G | N9-C4-C5 | -5.21 | 103.31 | 105.40 |
| 67 | 5 | 1690 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 67 | 5 | 1723 | A | C6-N1-C2 | -5.21 | 115.47 | 118.60 |
| 67 | 5 | 666 | G | N3-C4-C5 | 5.21 | 131.21 | 128.60 |
| 67 | 5 | 1911 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 67 | 5 | 4870 | G | N1-C2-N2 | -5.21 | 111.51 | 116.20 |
| 73 | 8 | 4 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 67 | 5 | 118 | C | C6-N1-C1' | -5.21 | 114.55 | 120.80 |
| 67 | 5 | 302 | C | C5-C4-N4 | -5.21 | 116.56 | 120.20 |
| 67 | 5 | 3783 | A | C5-N7-C8 | -5.21 | 101.30 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4279 | A | C5-N7-C8 | -5.21 | 101.30 | 103.90 |
| 67 | 5 | 4284 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 67 | 5 | 4503 | A | C6-N1-C2 | -5.21 | 115.48 | 118.60 |
| 75 | Z | 12 | LEU | CB-CG-CD2 | -5.21 | 102.15 | 111.00 |
| 76 | 9 | 1489 | A | O4'-C1'-N9 | 5.21 | 112.36 | 108.20 |
| 67 | 5 | 322 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 76 | 9 | 1014 | G | C4-N9-C1' | 5.21 | 133.27 | 126.50 |
| 52 | r | 20 | ARG | CG-CD-NE | 5.20 | 122.73 | 111.80 |
| 67 | 5 | 1989 | G | N3-C2-N2 | 5.20 | 123.54 | 119.90 |
| 67 | 5 | 3691 | G | O5'-P-OP1 | -5.20 | 101.02 | 105.70 |
| 67 | 5 | 4565 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 67 | 5 | 4230 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 67 | 5 | 140 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 67 | 5 | 1216 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 67 | 5 | 1630 | A | N1-C6-N6 | -5.20 | 115.48 | 118.60 |
| 67 | 5 | 1632 | A | N7-C8-N9 | 5.20 | 116.40 | 113.80 |
| 67 | 5 | 1786 | A | C8-N9-C4 | -5.20 | 103.72 | 105.80 |
| 67 | 5 | 3791 | C | C5-C4-N4 | -5.20 | 116.56 | 120.20 |
| 67 | 5 | 1343 | A | C5-C6-N1 | 5.20 | 120.30 | 117.70 |
| 67 | 5 | 4409 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 76 | 9 | 1413 | G | C4-N9-C1' | 5.20 | 133.26 | 126.50 |
| 67 | 5 | 1648 | C | C2-N1-C1' | 5.20 | 124.52 | 118.80 |
| 67 | 5 | 2348 | G | O4'-C1'-N9 | 5.20 | 112.36 | 108.20 |
| 67 | 5 | 1543 | G | N1-C2-N3 | 5.20 | 127.02 | 123.90 |
| 67 | 5 | 1554 | A | C5-C6-N1 | 5.20 | 120.30 | 117.70 |
| 67 | 5 | 1653 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 58 | t | 15 | LEU | CB-CG-CD1 | -5.19 | 102.17 | 111.00 |
| 67 | 5 | 1998 | A | C8-N9-C4 | -5.19 | 103.72 | 105.80 |
| 67 | 5 | 2533 | C | C5-C4-N4 | -5.19 | 116.56 | 120.20 |
| 67 | 5 | 3869 | C | N3-C4-C5 | 5.19 | 123.98 | 121.90 |
| 67 | 5 | 3923 | A | C5-C6-N6 | -5.19 | 119.55 | 123.70 |
| 67 | 5 | 4164 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 76 | 9 | 1146 | C | N3-C4-C5 | 5.19 | 123.98 | 121.90 |
| 67 | 5 | 2280 | G | C4-C5-N7 | 5.19 | 112.88 | 110.80 |
| 67 | 5 | 4603 | C | N3-C2-O2 | -5.19 | 118.27 | 121.90 |
| 67 | 5 | 112 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 67 | 5 | 1538 | U | O4'-C1'-N1 | 5.19 | 112.35 | 108.20 |
| 67 | 5 | 2278 | G | C4-N9-C1' | 5.19 | 133.25 | 126.50 |
| 67 | 5 | 2699 | C | C2-N1-C1' | 5.19 | 124.51 | 118.80 |
| 67 | 5 | 2772 | C | C6-N1-C1' | -5.19 | 114.57 | 120.80 |
| 67 | 5 | 3619 | G | C2-N3-C4 | -5.19 | 109.31 | 111.90 |
| 67 | 5 | 4217 | G | N3-C2-N2 | -5.19 | 116.27 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4630 | G | C8-N9-C4 | -5.19 | 104.32 | 106.40 |
| 76 | 9 | 1474 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 22 | HH | 61 | ILE | CG1-CB-CG2 | -5.19 | 99.99 | 111.40 |
| 24 | bb | 63 | LEU | CB-CG-CD1 | 5.19 | 119.82 | 111.00 |
| 67 | 5 | 2041 | A | N9-C4-C5 | 5.19 | 107.88 | 105.80 |
| 67 | 5 | 3903 | A | N9-C4-C5 | -5.19 | 103.72 | 105.80 |
| 76 | 9 | 1474 | A | C8-N9-C4 | -5.19 | 103.72 | 105.80 |
| 67 | 5 | 4253 | A | N1-C6-N6 | -5.19 | 115.49 | 118.60 |
| 67 | 5 | 4582 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 67 | 5 | 1065 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 67 | 5 | 1983 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 67 | 5 | 2438 | A | N9-C4-C5 | -5.18 | 103.73 | 105.80 |
| 67 | 5 | 2815 | A | N3-C4-N9 | 5.18 | 131.55 | 127.40 |
| 67 | 5 | 4971 | A | C6-C5-N7 | 5.18 | 135.93 | 132.30 |
| 67 | 5 | 1635 | C | C5-C4-N4 | -5.18 | 116.57 | 120.20 |
| 67 | 5 | 3834 | C | C6-N1-C1' | -5.18 | 114.58 | 120.80 |
| 73 | 8 | 88 | A | N1-C6-N6 | -5.18 | 115.49 | 118.60 |
| 76 | 9 | 1224 | G | C8-N9-C1' | 5.18 | 133.74 | 127.00 |
| 67 | 5 | 1465 | G | N1-C2-N2 | -5.18 | 111.54 | 116.20 |
| 67 | 5 | 2458 | C | C6-N1-C1' | -5.18 | 114.58 | 120.80 |
| 67 | 5 | 2629 | C | C6-N1-C1' | -5.18 | 114.58 | 120.80 |
| 67 | 5 | 2805 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 76 | 9 | 419 | G | C8-N9-C1' | -5.18 | 120.27 | 127.00 |
| 67 | 5 | 3719 | A | C6-C5-N7 | -5.18 | 128.68 | 132.30 |
| 67 | 5 | 1358 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 67 | 5 | 2040 | A | C8-N9-C1' | -5.18 | 118.38 | 127.70 |
| 67 | 5 | 4184 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 76 | 9 | 223 | C | C6-N1-C1' | -5.18 | 114.59 | 120.80 |
| 76 | 9 | 1849 | G | N7-C8-N9 | 5.18 | 115.69 | 113.10 |
| 67 | 5 | 2487 | G | C4-N9-C1' | 5.17 | 133.23 | 126.50 |
| 67 | 5 | 356 | G | C5-C6-N1 | -5.17 | 108.91 | 111.50 |
| 67 | 5 | 3653 | A | N3-C4-C5 | -5.17 | 123.18 | 126.80 |
| 76 | 9 | 1254 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 67 | 5 | 2295 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 76 | 9 | 1538 | C | O4'-C1'-N1 | 5.17 | 112.34 | 108.20 |
| 67 | 5 | 101 | A | C4-C5-N7 | 5.17 | 113.28 | 110.70 |
| 67 | 5 | 417 | G | C2-N3-C4 | -5.17 | 109.32 | 111.90 |
| 67 | 5 | 1484 | G | N1-C2-N2 | -5.17 | 111.55 | 116.20 |
| 67 | 5 | 1690 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 67 | 5 | 2349 | A | C5-N7-C8 | -5.17 | 101.32 | 103.90 |
| 67 | 5 | 2633 | U | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 67 | 5 | 3659 | G | C8-N9-C1' | -5.17 | 120.28 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4097 | G | N3-C4-N9 | -5.17 | 122.90 | 126.00 |
| 76 | 9 | 1181 | A | C5-N7-C8 | -5.17 | 101.31 | 103.90 |
| 67 | 5 | 418 | A | C5-N7-C8 | -5.17 | 101.32 | 103.90 |
| 67 | 5 | 2449 | A | C5-C6-N1 | 5.17 | 120.28 | 117.70 |
| 67 | 5 | 4688 | C | N3-C4-N4 | 5.17 | 121.62 | 118.00 |
| 76 | 9 | 1329 | U | O4'-C1'-N1 | -5.17 | 104.07 | 108.20 |
| 27 | II | 49 | ARG | CB-CG-CD | 5.16 | 125.03 | 111.60 |
| 67 | 5 | 1670 | G | N9-C4-C5 | -5.16 | 103.33 | 105.40 |
| 67 | 5 | 4171 | C | N3-C4-C5 | 5.16 | 123.97 | 121.90 |
| 67 | 5 | 4370 | G | C8-N9-C4 | -5.16 | 104.33 | 106.40 |
| 67 | 5 | 4687 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 67 | 5 | 1081 | C | N3-C4-N4 | 5.16 | 121.61 | 118.00 |
| 67 | 5 | 4427 | G | N3-C2-N2 | 5.16 | 123.51 | 119.90 |
| 67 | 5 | 4631 | G | N3-C4-C5 | -5.16 | 126.02 | 128.60 |
| 76 | 9 | 909 | G | C6-C5-N7 | -5.16 | 127.30 | 130.40 |
| 67 | 5 | 1305 | C | C6-N1-C1' | -5.16 | 114.61 | 120.80 |
| 67 | 5 | 1841 | C | C2-N1-C1' | 5.16 | 124.47 | 118.80 |
| 67 | 5 | 3899 | G | N7-C8-N9 | 5.16 | 115.68 | 113.10 |
| 67 | 5 | 4228 | G | N3-C4-C5 | -5.16 | 126.02 | 128.60 |
| 67 | 5 | 4878 | C | C6-N1-C1' | -5.16 | 114.61 | 120.80 |
| 67 | 5 | 4942 | C | C5-C4-N4 | 5.16 | 123.81 | 120.20 |
| 73 | 8 | 6 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 76 | 9 | 351 | G | N3-C2-N2 | -5.16 | 116.29 | 119.90 |
| 76 | 9 | 1224 | G | C4-N9-C1' | -5.16 | 119.79 | 126.50 |
| 67 | 5 | 1493 | G | C4-N9-C1' | 5.16 | 133.20 | 126.50 |
| 70 | 7 | 32 | A | C5-C6-N1 | 5.16 | 120.28 | 117.70 |
| 53 | QQ | 145 | TYR | CA-CB-CG | 5.16 | 123.19 | 113.40 |
| 67 | 5 | 2731 | C | C2-N1-C1' | 5.16 | 124.47 | 118.80 |
| 67 | 5 | 4462 | C | N3-C4-C5 | 5.16 | 123.96 | 121.90 |
| 67 | 5 | 4654 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 67 | 5 | 4694 | G | C8-N9-C1' | -5.16 | 120.30 | 127.00 |
| 76 | 9 | 1055 | A | C4-N9-C1' | 5.16 | 135.58 | 126.30 |
| 67 | 5 | 1929 | A | C6-C5-N7 | -5.15 | 128.69 | 132.30 |
| 76 | 9 | 533 | A | N9-C4-C5 | -5.15 | 103.74 | 105.80 |
| 67 | 5 | 4356 | G | C8-N9-C4 | -5.15 | 104.34 | 106.40 |
| 67 | 5 | 4478 | G | C8-N9-C1' | -5.15 | 120.30 | 127.00 |
| 76 | 9 | 1095 | U | C6-N1-C2 | -5.15 | 117.91 | 121.00 |
| 67 | 5 | 4630 | G | N7-C8-N9 | 5.15 | 115.67 | 113.10 |
| 67 | 5 | 1074 | G | C2-N3-C4 | -5.15 | 109.33 | 111.90 |
| 67 | 5 | 4195 | G | N1-C2-N3 | 5.15 | 126.99 | 123.90 |
| 67 | 5 | 4978 | G | C4-N9-C1' | 5.15 | 133.19 | 126.50 |
| 67 | 5 | 5059 | C | N3-C2-O2 | -5.15 | 118.30 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 2059 | C | C5-C4-N4 | -5.15 | 116.60 | 120.20 |
| 67 | 5 | 3864 | C | C5-C4-N4 | -5.15 | 116.60 | 120.20 |
| 22 | HH | 130 | LEU | CB-CG-CD2 | -5.14 | 102.25 | 111.00 |
| 67 | 5 | 3666 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 81 | B | 345 | LEU | CB-CG-CD1 | -5.14 | 102.26 | 111.00 |
| 67 | 5 | 19 | G | C4-N9-C1' | 5.14 | 133.19 | 126.50 |
| 67 | 5 | 1657 | G | N7-C8-N9 | 5.14 | 115.67 | 113.10 |
| 67 | 5 | 2081 | C | C5-C4-N4 | -5.14 | 116.60 | 120.20 |
| 67 | 5 | 2520 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 67 | 5 | 3913 | G | N1-C2-N2 | -5.14 | 111.57 | 116.20 |
| 67 | 5 | 52 | G | C4-N9-C1' | 5.14 | 133.18 | 126.50 |
| 76 | 9 | 1532 | C | C5-C6-N1 | 5.14 | 123.57 | 121.00 |
| 67 | 5 | 3623 | C | C2-N1-C1' | 5.14 | 124.45 | 118.80 |
| 67 | 5 | 2406 | G | N7-C8-N9 | 5.14 | 115.67 | 113.10 |
| 67 | 5 | 3668 | C | C2-N1-C1' | 5.14 | 124.45 | 118.80 |
| 67 | 5 | 108 | A | C8-N9-C1' | -5.14 | 118.45 | 127.70 |
| 67 | 5 | 1884 | C | N3-C2-O2 | -5.14 | 118.31 | 121.90 |
| 67 | 5 | 1966 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 67 | 5 | 2752 | G | C8-N9-C1' | -5.14 | 120.32 | 127.00 |
| 67 | 5 | 3706 | C | N3-C2-O2 | -5.14 | 118.31 | 121.90 |
| 67 | 5 | 4499 | G | C6-C5-N7 | -5.14 | 127.32 | 130.40 |
| 67 | 5 | 4525 | C | C6-N1-C1' | -5.14 | 114.64 | 120.80 |
| 67 | 5 | 1373 | A | C4-N9-C1' | 5.13 | 135.54 | 126.30 |
| 67 | 5 | 1729 | A | C5-C6-N6 | -5.13 | 119.59 | 123.70 |
| 76 | 9 | 909 | G | C4-N9-C1' | 5.13 | 133.17 | 126.50 |
| 67 | 5 | 47 | A | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 67 | 5 | 4330 | G | N1-C6-O6 | -5.13 | 116.82 | 119.90 |
| 76 | 9 | 70 | G | N3-C2-N2 | 5.13 | 123.49 | 119.90 |
| 67 | 5 | 1064 | G | C6-C5-N7 | -5.13 | 127.32 | 130.40 |
| 67 | 5 | 1541 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 15 | F | 73 | MET | CG-SD-CE | -5.13 | 92.00 | 100.20 |
| 37 | l | 49 | LEU | CB-CG-CD1 | -5.13 | 102.28 | 111.00 |
| 67 | 5 | 83 | C | C2-N3-C4 | -5.13 | 117.34 | 119.90 |
| 67 | 5 | 1661 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 67 | 5 | 2089 | G | C8-N9-C1' | -5.13 | 120.33 | 127.00 |
| 67 | 5 | 4391 | G | N1-C2-N2 | -5.13 | 111.58 | 116.20 |
| 67 | 5 | 4485 | C | C6-N1-C1' | -5.13 | 114.64 | 120.80 |
| 2 | C | 358 | LEU | CB-CG-CD2 | -5.13 | 102.29 | 111.00 |
| 67 | 5 | 1836 | G | N3-C2-N2 | 5.13 | 123.49 | 119.90 |
| 73 | 8 | 50 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 67 | 5 | 727 | C | C2-N1-C1' | 5.12 | 124.44 | 118.80 |
| 67 | 5 | 1298 | C | N3-C2-O2 | -5.12 | 118.31 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1896 | A | C6-C5-N7 | -5.12 | 128.71 | 132.30 |
| 67 | 5 | 2468 | U | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 67 | 5 | 3692 | A | C5-C6-N1 | 5.12 | 120.26 | 117.70 |
| 67 | 5 | 4338 | G | N3-C4-C5 | 5.12 | 131.16 | 128.60 |
| 23 | hh | 55 | C | O4'-C1'-N1 | 5.12 | 112.30 | 108.20 |
| 67 | 5 | 44 | A | C6-N1-C2 | -5.12 | 115.53 | 118.60 |
| 67 | 5 | 63 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 67 | 5 | 1329 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 67 | 5 | 4451 | G | N1-C2-N3 | 5.12 | 126.97 | 123.90 |
| 67 | 5 | 1875 | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 67 | 5 | 409 | G | C4-N9-C1' | 5.12 | 133.15 | 126.50 |
| 67 | 5 | 1988 | G | O4'-C1'-N9 | -5.12 | 104.11 | 108.20 |
| 67 | 5 | 4969 | C | C2-N1-C1' | 5.12 | 124.43 | 118.80 |
| 76 | 9 | 1456 | G | O4'-C1'-N9 | 5.12 | 112.30 | 108.20 |
| 67 | 5 | 241 | G | C8-N9-C1' | -5.12 | 120.35 | 127.00 |
| 67 | 5 | 1658 | G | C8-N9-C1' | -5.12 | 120.35 | 127.00 |
| 67 | 5 | 1662 | C | C5-C4-N4 | -5.12 | 116.62 | 120.20 |
| 67 | 5 | 4097 | G | O4'-C1'-N9 | -5.12 | 104.11 | 108.20 |
| 67 | 5 | 4761 | G | N3-C4-N9 | -5.12 | 122.93 | 126.00 |
| 67 | 5 | 973 | G | C8-N9-C4 | 5.11 | 108.44 | 106.40 |
| 67 | 5 | 4237 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 76 | 9 | 926 | A | O4'-C1'-N9 | 5.11 | 112.29 | 108.20 |
| 47 | OO | 27 | VAL | CG1-CB-CG2 | -5.11 | 102.72 | 110.90 |
| 67 | 5 | 197 | A | O4'-C1'-N9 | -5.11 | 104.11 | 108.20 |
| 67 | 5 | 2295 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 67 | 5 | 2397 | G | N1-C2-N3 | 5.11 | 126.97 | 123.90 |
| 73 | 8 | 44 | A | C5-N7-C8 | -5.11 | 101.34 | 103.90 |
| 76 | 9 | 561 | A | O4'-C1'-N9 | -5.11 | 104.11 | 108.20 |
| 4 | DD | 96 | LEU | CB-CG-CD2 | -5.11 | 102.32 | 111.00 |
| 67 | 5 | 2527 | A | N9-C4-C5 | 5.11 | 107.84 | 105.80 |
| 67 | 5 | 3857 | G | C6-C5-N7 | -5.11 | 127.34 | 130.40 |
| 67 | 5 | 2024 | G | C4-N9-C1' | -5.11 | 119.86 | 126.50 |
| 67 | 5 | 2737 | C | C6-N1-C1' | -5.11 | 114.67 | 120.80 |
| 67 | 5 | 1727 | U | C2-N1-C1' | 5.10 | 123.82 | 117.70 |
| 67 | 5 | 4623 | G | C4-N9-C1' | 5.10 | 133.13 | 126.50 |
| 23 | hh | 55 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 67 | 5 | 84 | A | N9-C4-C5 | -5.10 | 103.76 | 105.80 |
| 67 | 5 | 1330 | A | C5-C6-N1 | 5.10 | 120.25 | 117.70 |
| 67 | 5 | 2290 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 67 | 5 | 3717 | A | C5-C6-N6 | -5.10 | 119.62 | 123.70 |
| 67 | 5 | 3819 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 73 | 8 | 24 | G | N1-C2-N2 | -5.10 | 111.61 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | 9 | 1215 | C | O4'-C1'-N1 | 5.10 | 112.28 | 108.20 |
| 67 | 5 | 50 | C | C6-N1-C1' | -5.10 | 114.68 | 120.80 |
| 67 | 5 | 7 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 67 | 5 | 356 | G | C6-C5-N7 | -5.10 | 127.34 | 130.40 |
| 67 | 5 | 666 | G | C8-N9-C1' | 5.10 | 133.63 | 127.00 |
| 67 | 5 | 4568 | A | C6-N1-C2 | -5.10 | 115.54 | 118.60 |
| 73 | 8 | 41 | A | C8-N9-C1' | 5.10 | 136.88 | 127.70 |
| 76 | 9 | 1409 | A | O4'-C1'-N9 | 5.10 | 112.28 | 108.20 |
| 19 | gg | 258 | ILE | CG1-CB-CG2 | 5.10 | 122.61 | 111.40 |
| 70 | 7 | 48 | G | N9-C4-C5 | -5.10 | 103.36 | 105.40 |
| 76 | 9 | 356 | C | C2-N1-C1' | 5.10 | 124.41 | 118.80 |
| 67 | 5 | 747 | A | C5-N7-C8 | -5.10 | 101.35 | 103.90 |
| 67 | 5 | 4631 | G | N7-C8-N9 | 5.10 | 115.65 | 113.10 |
| 67 | 5 | 1607 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 67 | 5 | 2840 | A | C5-C6-N6 | -5.09 | 119.62 | 123.70 |
| 67 | 5 | 2846 | G | N3-C4-N9 | 5.09 | 129.06 | 126.00 |
| 67 | 5 | 3933 | G | C2-N3-C4 | -5.09 | 109.35 | 111.90 |
| 67 | 5 | 4392 | G | C5-C6-O6 | 5.09 | 131.66 | 128.60 |
| 73 | 8 | 126 | C | C6-N1-C1' | 5.09 | 126.91 | 120.80 |
| 76 | 9 | 1699 | A | N1-C6-N6 | 5.09 | 121.66 | 118.60 |
| 67 | 5 | 951 | G | C2-N3-C4 | -5.09 | 109.35 | 111.90 |
| 67 | 5 | 2622 | G | C6-C5-N7 | -5.09 | 127.34 | 130.40 |
| 67 | 5 | 360 | A | N7-C8-N9 | 5.09 | 116.35 | 113.80 |
| 67 | 5 | 1898 | C | C6-N1-C1' | -5.09 | 114.69 | 120.80 |
| 67 | 5 | 3873 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 76 | 9 | 677 | G | C8-N9-C1' | -5.09 | 120.39 | 127.00 |
| 76 | 9 | 1164 | G | C4-N9-C1' | 5.09 | 133.12 | 126.50 |
| 67 | 5 | 1648 | C | C6-N1-C1' | -5.09 | 114.69 | 120.80 |
| 67 | 5 | 1885 | G | C4-N9-C1' | 5.09 | 133.12 | 126.50 |
| 67 | 5 | 26 | C | N3-C4-N4 | 5.09 | 121.56 | 118.00 |
| 67 | 5 | 2003 | G | C4-N9-C1' | -5.09 | 119.89 | 126.50 |
| 67 | 5 | 2694 | G | C2-N3-C4 | -5.09 | 109.36 | 111.90 |
| 67 | 5 | 2724 | G | N3-C4-N9 | -5.09 | 122.95 | 126.00 |
| 67 | 5 | 4080 | C | N3-C2-O2 | -5.09 | 118.34 | 121.90 |
| 67 | 5 | 4169 | G | N1-C6-O6 | 5.09 | 122.95 | 119.90 |
| 67 | 5 | 4362 | A | N9-C4-C5 | 5.09 | 107.83 | 105.80 |
| 67 | 5 | 4370 | G | C4-N9-C1' | 5.09 | 133.11 | 126.50 |
| 67 | 5 | 1929 | A | C5-N7-C8 | -5.08 | 101.36 | 103.90 |
| 67 | 5 | 2297 | G | N3-C4-C5 | -5.08 | 126.06 | 128.60 |
| 67 | 5 | 4381 | A | C6-N1-C2 | -5.08 | 115.55 | 118.60 |
| 28 | ii | 88 | VAL | N-CA-C | -5.08 | 97.28 | 111.00 |
| 43 | n | 8 | LYS | CD-CE-NZ | 5.08 | 123.39 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4891 | G | N1-C2-N2 | -5.08 | 111.62 | 116.20 |
| 73 | 8 | 121 | G | N3-C4-C5 | 5.08 | 131.14 | 128.60 |
| 76 | 9 | 1630 | A | N1-C6-N6 | 5.08 | 121.65 | 118.60 |
| 67 | 5 | 63 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 67 | 5 | 2604 | C | C5-C4-N4 | -5.08 | 116.64 | 120.20 |
| 67 | 5 | 3812 | C | C6-N1-C1' | -5.08 | 114.70 | 120.80 |
| 67 | 5 | 3633 | C | C5-C4-N4 | -5.08 | 116.64 | 120.20 |
| 67 | 5 | 4561 | C | N3-C2-O2 | -5.08 | 118.34 | 121.90 |
| 67 | 5 | 414 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 67 | 5 | 1235 | G | N3-C4-C5 | 5.08 | 131.14 | 128.60 |
| 67 | 5 | 1363 | C | C5-C4-N4 | -5.08 | 116.64 | 120.20 |
| 67 | 5 | 1429 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 67 | 5 | 1586 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 67 | 5 | 1786 | A | C5-C6-N1 | 5.08 | 120.24 | 117.70 |
| 67 | 5 | 4196 | G | C8-N9-C4 | 5.08 | 108.43 | 106.40 |
| 67 | 5 | 4253 | A | C5-C6-N6 | 5.08 | 127.76 | 123.70 |
| 67 | 5 | 4971 | A | C8-N9-C1' | 5.08 | 136.84 | 127.70 |
| 73 | 8 | 90 | C | C6-N1-C1' | -5.08 | 114.71 | 120.80 |
| 76 | 9 | 196 | C | N3-C4-C5 | -5.08 | 119.87 | 121.90 |
| 76 | 9 | 1584 | G | O4'-C1'-N9 | -5.08 | 104.14 | 108.20 |
| 67 | 5 | 2284 | G | N1-C2-N2 | -5.08 | 111.63 | 116.20 |
| 76 | 9 | 845 | G | C4-N9-C1' | 5.08 | 133.10 | 126.50 |
| 67 | 5 | 343 | C | N3-C2-O2 | -5.08 | 118.35 | 121.90 |
| 67 | 5 | 1415 | G | C8-N9-C4 | 5.08 | 108.43 | 106.40 |
| 67 | 5 | 3774 | A | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 76 | 9 | 1243 | U | C6-N1-C1' | -5.08 | 114.09 | 121.20 |
| 6 | D | 212 | MET | CA-CB-CG | -5.07 | 104.68 | 113.30 |
| 67 | 5 | 156 | G | C2-N3-C4 | -5.07 | 109.36 | 111.90 |
| 67 | 5 | 3924 | C | C6-N1-C1' | -5.07 | 114.71 | 120.80 |
| 67 | 5 | 4193 | C | N3-C4-N4 | 5.07 | 121.55 | 118.00 |
| 67 | 5 | 4501 | U | O4'-C1'-N1 | 5.07 | 112.26 | 108.20 |
| 67 | 5 | 2275 | G | C8-N9-C1' | -5.07 | 120.41 | 127.00 |
| 67 | 5 | 4196 | G | C2-N3-C4 | -5.07 | 109.36 | 111.90 |
| 73 | 8 | 118 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 67 | 5 | 2448 | G | N7-C8-N9 | 5.07 | 115.63 | 113.10 |
| 67 | 5 | 1300 | G | C4-N9-C1' | -5.07 | 119.91 | 126.50 |
| 67 | 5 | 1928 | C | C2-N3-C4 | -5.07 | 117.37 | 119.90 |
| 67 | 5 | 1169 | G | N3-C4-C5 | 5.07 | 131.13 | 128.60 |
| 67 | 5 | 1972 | G | P-O3'-C3' | 5.07 | 125.78 | 119.70 |
| 67 | 5 | 4980 | C | C6-N1-C1' | -5.07 | 114.72 | 120.80 |
| 67 | 5 | 101 | A | C6-C5-N7 | -5.06 | 128.75 | 132.30 |
| 67 | 5 | 4538 | G | C4-C5-N7 | 5.06 | 112.83 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | 9 | 931 | C | C2-N1-C1' | 5.06 | 124.37 | 118.80 |
| 67 | 5 | 2469 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 67 | 5 | 2593 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 67 | 5 | 4213 | A | C8-N9-C1' | -5.06 | 118.59 | 127.70 |
| 67 | 5 | 4945 | G | C2-N3-C4 | -5.06 | 109.37 | 111.90 |
| 67 | 5 | 678 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 67 | 5 | 1603 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 25 | H | 168 | LYS | CB-CG-CD | 5.06 | 124.75 | 111.60 |
| 67 | 5 | 63 | G | N9-C4-C5 | -5.06 | 103.38 | 105.40 |
| 67 | 5 | 363 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 67 | 5 | 2505 | C | C2-N1-C1' | 5.06 | 124.37 | 118.80 |
| 67 | 5 | 2655 | C | N1-C2-O2 | 5.06 | 121.94 | 118.90 |
| 67 | 5 | 2860 | C | N1-C2-O2 | -5.06 | 115.86 | 118.90 |
| 67 | 5 | 3737 | A | C6-C5-N7 | -5.06 | 128.76 | 132.30 |
| 67 | 5 | 4170 | A | N1-C6-N6 | -5.06 | 115.56 | 118.60 |
| 76 | 9 | 1109 | C | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 76 | 9 | 1784 | G | C4-N9-C1' | 5.06 | 133.08 | 126.50 |
| 14 | ff | 146 | LEU | CB-CG-CD2 | 5.06 | 119.60 | 111.00 |
| 28 | ii | 188 | LEU | CB-CG-CD2 | 5.06 | 119.60 | 111.00 |
| 67 | 5 | 2280 | G | C5-N7-C8 | -5.06 | 101.77 | 104.30 |
| 76 | 9 | 213 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 76 | 9 | 1845 | A | C5-C6-N1 | 5.06 | 120.23 | 117.70 |
| 2 | C | 90 | GLY | N-CA-C | 5.05 | 125.74 | 113.10 |
| 28 | ii | 136 | LEU | CA-CB-CG | 5.05 | 126.93 | 115.30 |
| 67 | 5 | 1846 | G | N3-C2-N2 | 5.05 | 123.44 | 119.90 |
| 67 | 5 | 1859 | C | C2-N1-C1' | 5.05 | 124.36 | 118.80 |
| 67 | 5 | 2590 | G | N3-C2-N2 | 5.05 | 123.44 | 119.90 |
| 67 | 5 | 3670 | C | C5-C4-N4 | -5.05 | 116.66 | 120.20 |
| 67 | 5 | 2758 | G | N9-C4-C5 | -5.05 | 103.38 | 105.40 |
| 67 | 5 | 3877 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 67 | 5 | 4942 | C | N3-C4-N4 | -5.05 | 114.46 | 118.00 |
| 67 | 5 | 342 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 67 | 5 | 2411 | C | N3-C4-N4 | 5.05 | 121.54 | 118.00 |
| 67 | 5 | 2540 | C | C5-C6-N1 | 5.05 | 123.53 | 121.00 |
| 67 | 5 | 3665 | G | C4-N9-C1' | 5.05 | 133.07 | 126.50 |
| 67 | 5 | 4259 | C | C6-N1-C2 | -5.05 | 118.28 | 120.30 |
| 76 | 9 | 1834 | A | N1-C2-N3 | 5.05 | 131.83 | 129.30 |
| 76 | 9 | 1846 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 76 | 9 | 1856 | C | C2-N1-C1' | 5.05 | 124.36 | 118.80 |
| 67 | 5 | 2010 | A | C4-N9-C1' | -5.05 | 117.21 | 126.30 |
| 67 | 5 | 4195 | G | C8-N9-C1' | -5.05 | 120.44 | 127.00 |
| 67 | 5 | 4217 | G | N3-C4-N9 | -5.05 | 122.97 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 4613 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 67 | 5 | 4630 | G | C5-C6-O6 | 5.05 | 131.63 | 128.60 |
| 76 | 9 | 1000 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 76 | 9 | 84 | A | C5-C6-N1 | -5.05 | 115.18 | 117.70 |
| 67 | 5 | 108 | A | C6-C5-N7 | -5.05 | 128.77 | 132.30 |
| 67 | 5 | 375 | G | O4'-C1'-N9 | 5.05 | 112.24 | 108.20 |
| 67 | 5 | 3771 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 67 | 5 | 4980 | C | C6-N1-C2 | 5.05 | 122.32 | 120.30 |
| 67 | 5 | 1777 | C | C6-N1-C1' | -5.04 | 114.75 | 120.80 |
| 67 | 5 | 2691 | U | O4'-C1'-N1 | 5.04 | 112.24 | 108.20 |
| 76 | 9 | 476 | A | C5-C6-N6 | -5.04 | 119.67 | 123.70 |
| 76 | 9 | 329 | G | N3-C4-C5 | -5.04 | 126.08 | 128.60 |
| 76 | 9 | 1280 | G | C4-N9-C1' | 5.04 | 133.06 | 126.50 |
| 67 | 5 | 2320 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 76 | 9 | 1298 | G | O4'-C1'-N9 | -5.04 | 104.17 | 108.20 |
| 67 | 5 | 1346 | C | C5-C4-N4 | -5.04 | 116.67 | 120.20 |
| 67 | 5 | 1998 | A | N7-C8-N9 | 5.04 | 116.32 | 113.80 |
| 67 | 5 | 4669 | A | N3-C4-C5 | -5.04 | 123.27 | 126.80 |
| 76 | 9 | 1563 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 76 | 9 | 1617 | G | N3-C4-N9 | -5.04 | 122.98 | 126.00 |
| 67 | 5 | 3652 | A | C8-N9-C4 | -5.04 | 103.78 | 105.80 |
| 67 | 5 | 4458 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 67 | 5 | 1581 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 67 | 5 | 2000 | G | P-O3'-C3' | 5.04 | 125.74 | 119.70 |
| 76 | 9 | 168 | C | C6-N1-C1' | -5.04 | 114.76 | 120.80 |
| 67 | 5 | 3661 | G | N3-C2-N2 | 5.03 | 123.42 | 119.90 |
| 67 | 5 | 3936 | A | C6-N1-C2 | -5.03 | 115.58 | 118.60 |
| 67 | 5 | 289 | C | C6-N1-C1' | -5.03 | 114.76 | 120.80 |
| 67 | 5 | 2072 | C | C6-N1-C1' | -5.03 | 114.76 | 120.80 |
| 67 | 5 | 2271 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 67 | 5 | 421 | C | C2-N3-C4 | -5.03 | 117.39 | 119.90 |
| 67 | 5 | 1853 | G | C5-C6-N1 | -5.03 | 108.98 | 111.50 |
| 70 | 7 | 95 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 67 | 5 | 2487 | G | C8-N9-C1' | -5.03 | 120.46 | 127.00 |
| 76 | 9 | 845 | G | C8-N9-C1' | -5.03 | 120.46 | 127.00 |
| 67 | 5 | 343 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 67 | 5 | 386 | A | C4-N9-C1' | 5.03 | 135.35 | 126.30 |
| 67 | 5 | 3936 | A | C5-C6-N1 | 5.03 | 120.21 | 117.70 |
| 67 | 5 | 1581 | G | C6-C5-N7 | -5.02 | 127.39 | 130.40 |
| 67 | 5 | 4745 | G | O4'-C1'-N9 | 5.02 | 112.22 | 108.20 |
| 76 | 9 | 594 | A | N1-C6-N6 | -5.02 | 115.59 | 118.60 |
| 76 | 9 | 659 | G | C8-N9-C1' | -5.02 | 120.47 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 1812 | C | N3-C2-O2 | -5.02 | 118.39 | 121.90 |
| 67 | 5 | 2401 | A | C5-C6-N1 | 5.02 | 120.21 | 117.70 |
| 67 | 5 | 4391 | G | N1-C2-N3 | 5.02 | 126.91 | 123.90 |
| 67 | 5 | 4721 | G | C8-N9-C4 | -5.02 | 104.39 | 106.40 |
| 76 | 9 | 655 | A | N1-C6-N6 | 5.02 | 121.61 | 118.60 |
| 82 | c | 81 | LEU | CB-CG-CD2 | -5.02 | 102.47 | 111.00 |
| 67 | 5 | 1171 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 67 | 5 | 1330 | A | C6-N1-C2 | -5.02 | 115.59 | 118.60 |
| 67 | 5 | 1667 | A | C5-N7-C8 | -5.02 | 101.39 | 103.90 |
| 67 | 5 | 2271 | C | C6-N1-C1' | -5.02 | 114.78 | 120.80 |
| 67 | 5 | 1169 | G | C4-N9-C1' | -5.02 | 119.98 | 126.50 |
| 67 | 5 | 3751 | G | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 76 | 9 | 1293 | A | O4'-C1'-N9 | 5.02 | 112.21 | 108.20 |
| 67 | 5 | 711 | A | C5-C6-N1 | 5.01 | 120.21 | 117.70 |
| 67 | 5 | 2046 | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 67 | 5 | 3891 | A | C6-N1-C2 | -5.01 | 115.59 | 118.60 |
| 73 | 8 | 41 | A | C8-N9-C4 | -5.01 | 103.79 | 105.80 |
| 76 | 9 | 1302 | G | N3-C4-N9 | -5.01 | 122.99 | 126.00 |
| 76 | 9 | 1573 | G | C2-N3-C4 | -5.01 | 109.39 | 111.90 |
| 67 | 5 | 1331 | C | N3-C2-O2 | -5.01 | 118.39 | 121.90 |
| 67 | 5 | 1371 | A | C4-C5-N7 | 5.01 | 113.21 | 110.70 |
| 67 | 5 | 4543 | G | C8-N9-C1' | -5.01 | 120.48 | 127.00 |
| 67 | 5 | 5005 | G | N3-C4-C5 | 5.01 | 131.11 | 128.60 |
| 67 | 5 | 1663 | C | C6-N1-C1' | -5.01 | 114.79 | 120.80 |
| 67 | 5 | 2532 | C | C5-C4-N4 | -5.01 | 116.69 | 120.20 |
| 67 | 5 | 2772 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 67 | 5 | 4663 | G | C2-N3-C4 | -5.01 | 109.39 | 111.90 |
| 76 | 9 | 1826 | G | C4-N9-C1' | 5.01 | 133.02 | 126.50 |
| 67 | 5 | 1657 | G | N1-C2-N2 | -5.01 | 111.69 | 116.20 |
| 67 | 5 | 2324 | C | C6-N1-C1' | -5.01 | 114.79 | 120.80 |
| 67 | 5 | 2374 | A | C5-C6-N1 | 5.01 | 120.20 | 117.70 |
| 67 | 5 | 3696 | C | C6-N1-C1' | -5.01 | 114.79 | 120.80 |
| 67 | 5 | 3854 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 1 | A | 180 | LEU | CB-CG-CD2 | -5.01 | 102.49 | 111.00 |
| 67 | 5 | 64 | A | C6-C5-N7 | -5.01 | 128.79 | 132.30 |
| 67 | 5 | 4399 | U | O4'-C1'-N1 | 5.01 | 112.21 | 108.20 |
| 67 | 5 | 4880 | C | N3-C4-N4 | -5.01 | 114.49 | 118.00 |
| 67 | 5 | 1574 | G | C4-N9-C1' | 5.01 | 133.01 | 126.50 |
| 67 | 5 | 1755 | C | N1-C1'-C2' | 5.01 | 120.51 | 114.00 |
| 67 | 5 | 2694 | G | C4-N9-C1' | 5.01 | 133.01 | 126.50 |
| 67 | 5 | 2864 | A | C5-C6-N6 | -5.01 | 119.69 | 123.70 |
| 76 | 9 | 1470 | C | C6-N1-C2 | -5.00 | 118.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 67 | 5 | 165 | A | C5-C6-N6 | -5.00 | 119.70 | 123.70 |
| 67 | 5 | 1585 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 67 | 5 | 1893 | C | C2-N1-C1' | 5.00 | 124.30 | 118.80 |
| 76 | 9 | 18 | C | C2-N1-C1' | 5.00 | 124.30 | 118.80 |
| 67 | 5 | 2040 | A | C4-N9-C1' | 5.00 | 135.30 | 126.30 |
| 67 | 5 | 2078 | C | N3-C4-N4 | 5.00 | 121.50 | 118.00 |
| 67 | 5 | 2604 | C | N1-C2-O2 | 5.00 | 121.90 | 118.90 |
| 67 | 5 | 2895 | A | N1-C6-N6 | 5.00 | 121.60 | 118.60 |
| 67 | 5 | 3614 | G | O4'-C1'-N9 | 5.00 | 112.20 | 108.20 |
| 67 | 5 | 3895 | G | C8-N9-C4 | -5.00 | 104.40 | 106.40 |
| 67 | 5 | 4367 | G | N3-C2-N2 | 5.00 | 123.40 | 119.90 |
| 76 | 9 | 141 | A | N1-C6-N6 | -5.00 | 115.60 | 118.60 |
| 76 | 9 | 1167 | G | C4-N9-C1' | 5.00 | 133.00 | 126.50 |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 67 | 5 | 1081 | C | Sidechain |
| 67 | 5 | 1576 | G | Sidechain |
| 67 | 5 | 1632 | A | Sidechain |
| 67 | 5 | 3623 | C | Sidechain |
| 67 | 5 | 3653 | A | Sidechain |
| 67 | 5 | 39 | A | Sidechain |
| 67 | 5 | 914 | U | Sidechain |
| 76 | 9 | 140 | U | Sidechain |
| 79 | AA | 42 | LYS | Peptide |
| 53 | QQ | 140 | ARG | Peptide |
| 71 | XX | 61 | GLN | Peptide |
| 3 | d | 95 | ASP | Peptide |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 246/249 (99%) | 219 (89%) | 27 (11%) | 0 | 100 | 100 |
| 2 | C | 360/378 (95%) | 335 (93%) | 24 (7%) | 1 (0%) | 41 | 75 |
| 3 | d | 105/108 (97%) | 90 (86%) | 13 (12%) | 2 (2%) | 8 | 39 |
| 4 | DD | 226/281 (80%) | 212 (94%) | 13 (6%) | 1 (0%) | 34 | 71 |
| 5 | dd | 53/56 (95%) | 46 (87%) | 7 (13%) | 0 | 100 | 100 |
| 6 | D | 291/296 (98%) | 273 (94%) | 18 (6%) | 0 | 100 | 100 |
| 7 | e | 126/129 (98%) | 121 (96%) | 5 (4%) | 0 | 100 | 100 |
| 8 | EE | 260/263 (99%) | 244 (94%) | 16 (6%) | 0 | 100 | 100 |
| 9 | ee | 53/133 (40%) | 51 (96%) | 2 (4%) | 0 | 100 | 100 |
| 10 | b | 100/226 (44%) | 94 (94%) | 5 (5%) | 1 (1%) | 15 | 52 |
| 11 | E | 208/291 (72%) | 189 (91%) | 19 (9%) | 0 | 100 | 100 |
| 12 | f | 107/110 (97%) | 98 (92%) | 7 (6%) | 2 (2%) | 8 | 39 |
| 13 | FF | 181/204 (89%) | 164 (91%) | 14 (8%) | 3 (2%) | 9 | 42 |
| 14 | ff | 66/68 (97%) | 62 (94%) | 4 (6%) | 0 | 100 | 100 |
| 15 | F | 223/249 (90%) | 213 (96%) | 9 (4%) | 1 (0%) | 34 | 71 |
| 16 | g | 112/126 (89%) | 106 (95%) | 6 (5%) | 0 | 100 | 100 |
| 17 | BB | 211/264 (80%) | 193 (92%) | 18 (8%) | 0 | 100 | 100 |
| 18 | GG | 235/263 (89%) | 223 (95%) | 12 (5%) | 0 | 100 | 100 |
| 19 | gg | 311/314 (99%) | 282 (91%) | 27 (9%) | 2 (1%) | 25 | 63 |
| 20 | G | 229/242 (95%) | 218 (95%) | 9 (4%) | 2 (1%) | 17 | 54 |
| 21 | h | 120/123 (98%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 22 | HH | 181/191 (95%) | 173 (96%) | 8 (4%) | 0 | 100 | 100 |
| 24 | bb | 81/84 (96%) | 74 (91%) | 7 (9%) | 0 | 100 | 100 |
| 25 | H | 188/190 (99%) | 178 (95%) | 10 (5%) | 0 | 100 | 100 |
| 26 | i | 100/107 (94%) | 94 (94%) | 6 (6%) | 0 | 100 | 100 |
| 27 | II | 204/208 (98%) | 188 (92%) | 14 (7%) | 2 (1%) | 15 | 52 |
| 28 | ii | 417/437 (95%) | 389 (93%) | 24 (6%) | 4 (1%) | 15 | 52 |
| 29 | I | 201/214 (94%) | 182 (90%) | 19 (10%) | 0 | 100 | 100 |
| 30 | j | 84/97 (87%) | 78 (93%) | 6 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 31 | JJ | 183/194 (94%) | 177 (97%) | 6 (3%) | 0 | 100 | 100 |
| 32 | jj | 426/428 (100%) | 373 (88%) | 46 (11%) | 7 (2%) | 9 | 43 |
| 33 | J | 168/176 (96%) | 160 (95%) | 8 (5%) | 0 | 100 | 100 |
| 34 | k | 67/70 (96%) | 63 (94%) | 4 (6%) | 0 | 100 | 100 |
| 35 | KK | 94/151 (62%) | 88 (94%) | 5 (5%) | 1 (1%) | 14 | 50 |
| 36 | L | 208/211 (99%) | 192 (92%) | 15 (7%) | 1 (0%) | 29 | 67 |
| 37 | l | 48/51 (94%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 38 | LL | 139/158 (88%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 39 | M | 136/218 (62%) | 123 (90%) | 13 (10%) | 0 | 100 | 100 |
| 40 | m | 50/128 (39%) | 46 (92%) | 4 (8%) | 0 | 100 | 100 |
| 41 | MM | 115/123 (94%) | 103 (90%) | 12 (10%) | 0 | 100 | 100 |
| 42 | N | 201/204 (98%) | 186 (92%) | 11 (6%) | 4 (2%) | 7 | 39 |
| 43 | n | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 44 | NN | 147/150 (98%) | 140 (95%) | 6 (4%) | 1 (1%) | 22 | 60 |
| 45 | O | 197/203 (97%) | 189 (96%) | 7 (4%) | 1 (0%) | 29 | 67 |
| 46 | o | 102/142 (72%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 47 | OO | 134/156 (86%) | 124 (92%) | 8 (6%) | 2 (2%) | 10 | 44 |
| 48 | P | 151/199 (76%) | 143 (95%) | 8 (5%) | 0 | 100 | 100 |
| 49 | p | 89/109 (82%) | 82 (92%) | 7 (8%) | 0 | 100 | 100 |
| 50 | PP | 118/145 (81%) | 104 (88%) | 12 (10%) | 2 (2%) | 9 | 42 |
| 51 | Q | 185/188 (98%) | 173 (94%) | 11 (6%) | 1 (0%) | 29 | 67 |
| 52 | r | 122/137 (89%) | 112 (92%) | 9 (7%) | 1 (1%) | 19 | 58 |
| 53 | QQ | 140/158 (89%) | 133 (95%) | 6 (4%) | 1 (1%) | 22 | 60 |
| 54 | R | 178/196 (91%) | 173 (97%) | 5 (3%) | 0 | 100 | 100 |
| 55 | s | 194/318 (61%) | 175 (90%) | 17 (9%) | 2 (1%) | 15 | 52 |
| 56 | RR | 130/145 (90%) | 121 (93%) | 9 (7%) | 0 | 100 | 100 |
| 57 | S | 174/176 (99%) | 159 (91%) | 12 (7%) | 3 (2%) | 9 | 42 |
| 58 | t | 151/196 (77%) | 134 (89%) | 16 (11%) | 1 (1%) | 22 | 60 |
| 59 | SS | 142/152 (93%) | 137 (96%) | 4 (3%) | 1 (1%) | 22 | 60 |
| 60 | T | 157/160 (98%) | 146 (93%) | 11 (7%) | 0 | 100 | 100 |
| 61 | TT | 139/145 (96%) | 131 (94%) | 8 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 62 | U | 97/128 (76%) | 89 (92%) | 8 (8%) | 0 | 100 100 |
| 63 | UU | 98/118 (83%) | 91 (93%) | 7 (7%) | 0 | 100 100 |
| 64 | V | 129/132 (98%) | 119 (92%) | 10 (8%) | 0 | 100 100 |
| 65 | VV | 81/83 (98%) | 78 (96%) | 3 (4%) | 0 | 100 100 |
| 66 | W | 102/134 (76%) | 98 (96%) | 4 (4%) | 0 | 100 100 |
| 68 | WW | 127/139 (91%) | 118 (93%) | 7 (6%) | 2 (2%) | 9 43 |
| 69 | X | 116/156 (74%) | 107 (92%) | 9 (8%) | 0 | 100 100 |
| 71 | XX | 139/142 (98%) | 125 (90%) | 11 (8%) | 3 (2%) | 6 37 |
| 72 | Y | 132/134 (98%) | 121 (92%) | 11 (8%) | 0 | 100 100 |
| 74 | YY | 122/146 (84%) | 115 (94%) | 7 (6%) | 0 | 100 100 |
| 75 | Z | 133/136 (98%) | 125 (94%) | 6 (4%) | 2 (2%) | 10 44 |
| 77 | ZZ | 73/122 (60%) | 69 (94%) | 4 (6%) | 0 | 100 100 |
| 78 | a | 145/147 (99%) | 129 (89%) | 16 (11%) | 0 | 100 100 |
| 79 | AA | 215/295 (73%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 67 |
| 80 | aa | 99/117 (85%) | 89 (90%) | 9 (9%) | 1 (1%) | 15 52 |
| 81 | B | 392/402 (98%) | 355 (91%) | 35 (9%) | 2 (0%) | 29 67 |
| 82 | c | 96/115 (84%) | 94 (98%) | 2 (2%) | 0 | 100 100 |
| 83 | CC | 219/259 (85%) | 205 (94%) | 14 (6%) | 0 | 100 100 |
| 84 | cc | 60/69 (87%) | 58 (97%) | 2 (3%) | 0 | 100 100 |
| All | All | 12362/14087 (88%) | 11478 (93%) | 823 (7%) | 61 (0%) | 32 67 |

All (61) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 95 | ASP |
| 28 | ii | 272 | THR |
| 32 | jj | 466 | LYS |
| 32 | jj | 620 | GLU |
| 42 | N | 76 | PRO |
| 42 | N | 77 | LYS |
| 50 | PP | 18 | ARG |
| 71 | XX | 62 | PRO |
| 71 | XX | 86 | PRO |
| 27 | II | 124 | LYS |
| 28 | ii | 181 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 28 | ii | 258 | TYR |
| 32 | jj | 224 | GLY |
| 32 | jj | 280 | VAL |
| 32 | jj | 555 | HIS |
| 44 | NN | 108 | ASP |
| 45 | O | 186 | GLU |
| 52 | r | 11 | ARG |
| 53 | QQ | 30 | GLY |
| 59 | SS | 100 | ALA |
| 10 | b | 102 | PRO |
| 12 | f | 107 | PRO |
| 28 | ii | 370 | GLU |
| 35 | KK | 64 | TRP |
| 36 | L | 63 | THR |
| 42 | N | 89 | VAL |
| 47 | OO | 20 | GLN |
| 47 | OO | 30 | VAL |
| 55 | s | 142 | GLY |
| 57 | S | 155 | PRO |
| 75 | Z | 91 | LEU |
| 80 | aa | 99 | PRO |
| 13 | FF | 43 | GLU |
| 13 | FF | 80 | GLY |
| 50 | PP | 80 | LEU |
| 57 | S | 166 | ARG |
| 58 | t | 125 | LEU |
| 68 | WW | 56 | HIS |
| 71 | XX | 61 | GLN |
| 75 | Z | 90 | PRO |
| 4 | DD | 93 | THR |
| 12 | f | 106 | TYR |
| 57 | S | 53 | LYS |
| 81 | B | 17 | LEU |
| 81 | B | 376 | HIS |
| 15 | F | 196 | VAL |
| 32 | jj | 558 | ILE |
| 42 | N | 55 | ALA |
| 79 | AA | 159 | ILE |
| 13 | FF | 21 | GLY |
| 19 | gg | 224 | GLY |
| 55 | s | 25 | PRO |
| 68 | WW | 29 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | d | 58 | GLY |
| 27 | II | 3 | ILE |
| 19 | gg | 275 | ILE |
| 20 | G | 216 | PRO |
| 51 | Q | 92 | VAL |
| 2 | C | 83 | GLY |
| 20 | G | 221 | VAL |
| 32 | jj | 464 | ILE |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | A | 190/191 (100%) | 188 (99%) | 2 (1%) | 73 84 |
| 2 | C | 302/315 (96%) | 301 (100%) | 1 (0%) | 92 95 |
| 3 | d | 98/99 (99%) | 97 (99%) | 1 (1%) | 76 85 |
| 4 | DD | 190/232 (82%) | 185 (97%) | 5 (3%) | 46 67 |
| 5 | dd | 48/49 (98%) | 48 (100%) | 0 | 100 100 |
| 6 | D | 247/249 (99%) | 245 (99%) | 2 (1%) | 81 88 |
| 7 | e | 114/115 (99%) | 113 (99%) | 1 (1%) | 78 87 |
| 8 | EE | 224/225 (100%) | 223 (100%) | 1 (0%) | 91 94 |
| 9 | ee | 46/106 (43%) | 46 (100%) | 0 | 100 100 |
| 10 | b | 84/172 (49%) | 84 (100%) | 0 | 100 100 |
| 11 | E | 190/251 (76%) | 186 (98%) | 4 (2%) | 53 72 |
| 12 | f | 88/89 (99%) | 87 (99%) | 1 (1%) | 73 84 |
| 13 | FF | 158/170 (93%) | 157 (99%) | 1 (1%) | 86 92 |
| 14 | ff | 61/61 (100%) | 59 (97%) | 2 (3%) | 38 62 |
| 15 | F | 196/218 (90%) | 195 (100%) | 1 (0%) | 88 93 |
| 16 | g | 98/106 (92%) | 97 (99%) | 1 (1%) | 76 85 |
| 17 | BB | 194/229 (85%) | 192 (99%) | 2 (1%) | 76 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 18 | GG | 207/228 (91%) | 204 (99%) | 3 (1%) | 67 80 |
| 19 | gg | 272/273 (100%) | 270 (99%) | 2 (1%) | 84 90 |
| 20 | G | 200/207 (97%) | 200 (100%) | 0 | 100 100 |
| 21 | h | 109/110 (99%) | 108 (99%) | 1 (1%) | 78 87 |
| 22 | HH | 165/171 (96%) | 164 (99%) | 1 (1%) | 86 92 |
| 24 | bb | 75/76 (99%) | 74 (99%) | 1 (1%) | 69 81 |
| 25 | H | 169/169 (100%) | 168 (99%) | 1 (1%) | 86 92 |
| 26 | i | 86/88 (98%) | 86 (100%) | 0 | 100 100 |
| 27 | II | 178/180 (99%) | 173 (97%) | 5 (3%) | 43 65 |
| 28 | ii | 361/376 (96%) | 358 (99%) | 3 (1%) | 81 88 |
| 29 | I | 175/181 (97%) | 174 (99%) | 1 (1%) | 86 92 |
| 30 | j | 73/80 (91%) | 72 (99%) | 1 (1%) | 67 80 |
| 31 | JJ | 161/168 (96%) | 159 (99%) | 2 (1%) | 71 83 |
| 32 | jj | 372/372 (100%) | 363 (98%) | 9 (2%) | 49 69 |
| 33 | J | 143/148 (97%) | 141 (99%) | 2 (1%) | 67 80 |
| 34 | k | 64/65 (98%) | 64 (100%) | 0 | 100 100 |
| 35 | KK | 87/127 (68%) | 86 (99%) | 1 (1%) | 73 84 |
| 36 | L | 175/176 (99%) | 174 (99%) | 1 (1%) | 86 92 |
| 37 | l | 47/48 (98%) | 46 (98%) | 1 (2%) | 53 72 |
| 38 | LL | 130/143 (91%) | 128 (98%) | 2 (2%) | 65 79 |
| 39 | M | 117/161 (73%) | 112 (96%) | 5 (4%) | 29 56 |
| 40 | m | 48/116 (41%) | 48 (100%) | 0 | 100 100 |
| 41 | MM | 99/104 (95%) | 98 (99%) | 1 (1%) | 76 85 |
| 42 | N | 171/172 (99%) | 168 (98%) | 3 (2%) | 59 77 |
| 43 | n | 24/24 (100%) | 24 (100%) | 0 | 100 100 |
| 44 | NN | 130/131 (99%) | 127 (98%) | 3 (2%) | 50 70 |
| 45 | O | 171/173 (99%) | 168 (98%) | 3 (2%) | 59 77 |
| 46 | o | 92/121 (76%) | 92 (100%) | 0 | 100 100 |
| 47 | OO | 106/122 (87%) | 104 (98%) | 2 (2%) | 57 75 |
| 48 | P | 134/175 (77%) | 133 (99%) | 1 (1%) | 84 90 |
| 49 | p | 74/87 (85%) | 73 (99%) | 1 (1%) | 67 80 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 50 | PP | 109/130 (84%) | 108 (99%) | 1 (1%) | 78 87 |
| 51 | Q | 164/165 (99%) | 163 (99%) | 1 (1%) | 86 92 |
| 52 | r | 108/121 (89%) | 104 (96%) | 4 (4%) | 34 59 |
| 53 | QQ | 117/130 (90%) | 117 (100%) | 0 | 100 100 |
| 54 | R | 159/175 (91%) | 157 (99%) | 2 (1%) | 69 81 |
| 55 | s | 164/258 (64%) | 162 (99%) | 2 (1%) | 71 83 |
| 56 | RR | 119/131 (91%) | 117 (98%) | 2 (2%) | 60 78 |
| 57 | S | 157/157 (100%) | 155 (99%) | 2 (1%) | 69 81 |
| 58 | t | 126/164 (77%) | 124 (98%) | 2 (2%) | 62 78 |
| 59 | SS | 125/132 (95%) | 123 (98%) | 2 (2%) | 62 78 |
| 60 | T | 139/140 (99%) | 138 (99%) | 1 (1%) | 84 90 |
| 61 | TT | 111/115 (96%) | 110 (99%) | 1 (1%) | 78 87 |
| 62 | U | 89/114 (78%) | 89 (100%) | 0 | 100 100 |
| 63 | UU | 92/105 (88%) | 90 (98%) | 2 (2%) | 52 71 |
| 64 | V | 101/102 (99%) | 97 (96%) | 4 (4%) | 31 57 |
| 65 | VV | 67/67 (100%) | 64 (96%) | 3 (4%) | 27 54 |
| 66 | W | 86/109 (79%) | 84 (98%) | 2 (2%) | 50 70 |
| 68 | WW | 112/119 (94%) | 110 (98%) | 2 (2%) | 59 77 |
| 69 | X | 106/134 (79%) | 106 (100%) | 0 | 100 100 |
| 71 | XX | 113/114 (99%) | 112 (99%) | 1 (1%) | 78 87 |
| 72 | Y | 124/124 (100%) | 124 (100%) | 0 | 100 100 |
| 74 | YY | 107/126 (85%) | 105 (98%) | 2 (2%) | 57 75 |
| 75 | Z | 117/118 (99%) | 116 (99%) | 1 (1%) | 78 87 |
| 77 | ZZ | 66/100 (66%) | 65 (98%) | 1 (2%) | 65 79 |
| 78 | a | 119/119 (100%) | 119 (100%) | 0 | 100 100 |
| 79 | AA | 180/245 (74%) | 177 (98%) | 3 (2%) | 60 78 |
| 80 | aa | 88/99 (89%) | 87 (99%) | 1 (1%) | 73 84 |
| 81 | B | 342/347 (99%) | 340 (99%) | 2 (1%) | 86 92 |
| 82 | c | 84/98 (86%) | 84 (100%) | 0 | 100 100 |
| 83 | CC | 187/208 (90%) | 185 (99%) | 2 (1%) | 73 84 |
| 84 | cc | 55/62 (89%) | 54 (98%) | 1 (2%) | 59 77 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| All | All | 10776/11977 (90%) | 10648 (99%) | 128 (1%) | 72 83 |

All (128) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 102 | LEU |
| 1 | A | 128 | ARG |
| 2 | C | 188 | ARG |
| 3 | d | 31 | LYS |
| 4 | DD | 76 | ARG |
| 4 | DD | 90 | LYS |
| 4 | DD | 156 | LEU |
| 4 | DD | 167 | TYR |
| 4 | DD | 218 | LEU |
| 6 | D | 37 | VAL |
| 6 | D | 56 | THR |
| 7 | e | 89 | LEU |
| 8 | EE | 49 | ARG |
| 11 | E | 141 | ARG |
| 11 | E | 144 | ARG |
| 11 | E | 242 | LYS |
| 11 | E | 289 | LEU |
| 12 | f | 47 | CYS |
| 13 | FF | 169 | ILE |
| 14 | ff | 99 | LYS |
| 14 | ff | 138 | ARG |
| 15 | F | 30 | LYS |
| 16 | g | 102 | ILE |
| 17 | BB | 38 | MET |
| 17 | BB | 207 | LEU |
| 18 | GG | 103 | ASP |
| 18 | GG | 137 | ARG |
| 18 | GG | 178 | ARG |
| 19 | gg | 289 | LEU |
| 19 | gg | 306 | LEU |
| 21 | h | 28 | LEU |
| 22 | HH | 194 | LEU |
| 24 | bb | 37 | CYS |
| 25 | H | 74 | CYS |
| 27 | II | 12 | ARG |
| 27 | II | 76 | THR |
| 27 | II | 100 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | II | 130 | THR |
| 27 | II | 205 | ARG |
| 28 | ii | 63 | LYS |
| 28 | ii | 171 | LYS |
| 28 | ii | 291 | PHE |
| 29 | I | 153 | ARG |
| 30 | j | 58 | THR |
| 31 | JJ | 50 | LEU |
| 31 | JJ | 112 | THR |
| 32 | jj | 249 | ARG |
| 32 | jj | 353 | LEU |
| 32 | jj | 371 | ARG |
| 32 | jj | 384 | LYS |
| 32 | jj | 455 | VAL |
| 32 | jj | 541 | LYS |
| 32 | jj | 551 | VAL |
| 32 | jj | 581 | ARG |
| 32 | jj | 631 | LYS |
| 33 | J | 16 | ARG |
| 33 | J | 58 | ARG |
| 35 | KK | 20 | VAL |
| 36 | L | 10 | LEU |
| 37 | l | 49 | LEU |
| 38 | LL | 33 | LEU |
| 38 | LL | 69 | ARG |
| 39 | M | 5 | ARG |
| 39 | M | 37 | LEU |
| 39 | M | 54 | CYS |
| 39 | M | 57 | LEU |
| 39 | M | 119 | ARG |
| 41 | MM | 31 | LEU |
| 42 | N | 26 | ARG |
| 42 | N | 27 | CYS |
| 42 | N | 162 | ARG |
| 44 | NN | 20 | ARG |
| 44 | NN | 84 | LEU |
| 44 | NN | 107 | LYS |
| 45 | O | 9 | LEU |
| 45 | O | 145 | VAL |
| 45 | O | 156 | LEU |
| 47 | OO | 98 | ARG |
| 47 | OO | 119 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 48 | P | 128 | ARG |
| 49 | p | 8 | VAL |
| 50 | PP | 44 | ARG |
| 51 | Q | 97 | LYS |
| 52 | r | 32 | LEU |
| 52 | r | 35 | ARG |
| 52 | r | 80 | THR |
| 52 | r | 103 | HIS |
| 54 | R | 74 | ARG |
| 54 | R | 133 | LYS |
| 55 | s | 95 | LEU |
| 55 | s | 187 | LEU |
| 56 | RR | 30 | THR |
| 56 | RR | 35 | CYS |
| 57 | S | 69 | GLU |
| 57 | S | 174 | THR |
| 58 | t | 90 | ARG |
| 58 | t | 99 | LYS |
| 59 | SS | 52 | LEU |
| 59 | SS | 59 | LEU |
| 60 | T | 146 | LYS |
| 61 | TT | 121 | ARG |
| 63 | UU | 55 | ARG |
| 63 | UU | 88 | LEU |
| 64 | V | 18 | LEU |
| 64 | V | 35 | LYS |
| 64 | V | 48 | ARG |
| 64 | V | 82 | ILE |
| 65 | VV | 11 | LEU |
| 65 | VV | 66 | ASP |
| 65 | VV | 68 | SER |
| 66 | W | 17 | HIS |
| 66 | W | 110 | ARG |
| 68 | WW | 20 | ARG |
| 68 | WW | 104 | LEU |
| 71 | XX | 82 | THR |
| 74 | YY | 79 | LEU |
| 74 | YY | 110 | ARG |
| 75 | Z | 33 | THR |
| 77 | ZZ | 77 | LEU |
| 79 | AA | 58 | LEU |
| 79 | AA | 111 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 79 | AA | 163 | CYS |
| 80 | aa | 21 | ILE |
| 81 | B | 248 | LEU |
| 81 | B | 261 | ARG |
| 83 | CC | 78 | LEU |
| 83 | CC | 114 | LYS |
| 84 | cc | 40 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 187 | HIS |
| 2 | C | 212 | ASN |
| 2 | C | 245 | HIS |
| 5 | dd | 3 | HIS |
| 5 | dd | 28 | HIS |
| 6 | D | 175 | HIS |
| 6 | D | 222 | GLN |
| 7 | e | 57 | ASN |
| 10 | b | 12 | GLN |
| 11 | E | 45 | HIS |
| 11 | E | 131 | HIS |
| 11 | E | 214 | HIS |
| 11 | E | 253 | GLN |
| 11 | E | 269 | GLN |
| 12 | f | 24 | HIS |
| 12 | f | 99 | HIS |
| 13 | FF | 31 | ASN |
| 13 | FF | 65 | GLN |
| 13 | FF | 101 | HIS |
| 13 | FF | 107 | ASN |
| 13 | FF | 148 | ASN |
| 13 | FF | 149 | GLN |
| 13 | FF | 203 | ASN |
| 14 | ff | 91 | ASN |
| 15 | F | 57 | HIS |
| 15 | F | 79 | ASN |
| 15 | F | 191 | HIS |
| 15 | F | 199 | HIS |
| 16 | g | 114 | GLN |
| 17 | BB | 118 | GLN |
| 17 | BB | 124 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | BB | 186 | ASN |
| 18 | GG | 59 | GLN |
| 18 | GG | 81 | HIS |
| 18 | GG | 146 | ASN |
| 19 | gg | 4 | GLN |
| 19 | gg | 14 | HIS |
| 19 | gg | 147 | HIS |
| 19 | gg | 159 | ASN |
| 20 | G | 82 | ASN |
| 20 | G | 138 | GLN |
| 20 | G | 206 | GLN |
| 22 | HH | 76 | GLN |
| 22 | HH | 97 | GLN |
| 22 | HH | 165 | ASN |
| 24 | bb | 26 | GLN |
| 25 | H | 15 | ASN |
| 25 | H | 78 | GLN |
| 25 | H | 156 | ASN |
| 26 | i | 15 | HIS |
| 26 | i | 20 | ASN |
| 27 | II | 99 | ASN |
| 28 | ii | 132 | HIS |
| 28 | ii | 247 | GLN |
| 28 | ii | 356 | HIS |
| 29 | I | 73 | ASN |
| 31 | JJ | 124 | HIS |
| 31 | JJ | 134 | HIS |
| 31 | JJ | 140 | GLN |
| 32 | jj | 212 | HIS |
| 32 | jj | 214 | ASN |
| 32 | jj | 220 | HIS |
| 32 | jj | 255 | ASN |
| 32 | jj | 410 | GLN |
| 32 | jj | 468 | GLN |
| 32 | jj | 534 | GLN |
| 32 | jj | 540 | HIS |
| 35 | KK | 39 | ASN |
| 35 | KK | 42 | ASN |
| 35 | KK | 61 | GLN |
| 35 | KK | 66 | HIS |
| 36 | L | 87 | HIS |
| 37 | l | 4 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | LL | 5 | GLN |
| 38 | LL | 18 | GLN |
| 38 | LL | 39 | ASN |
| 38 | LL | 141 | ASN |
| 39 | M | 131 | GLN |
| 40 | m | 93 | ASN |
| 41 | MM | 28 | HIS |
| 41 | MM | 48 | HIS |
| 42 | N | 15 | GLN |
| 42 | N | 196 | ASN |
| 42 | N | 201 | HIS |
| 44 | NN | 138 | ASN |
| 45 | O | 50 | ASN |
| 45 | O | 72 | HIS |
| 45 | O | 180 | GLN |
| 46 | o | 18 | HIS |
| 46 | o | 36 | GLN |
| 47 | OO | 43 | HIS |
| 47 | OO | 79 | GLN |
| 48 | P | 25 | HIS |
| 48 | P | 28 | ASN |
| 48 | P | 34 | GLN |
| 48 | P | 56 | GLN |
| 48 | P | 75 | GLN |
| 48 | P | 116 | HIS |
| 48 | P | 120 | ASN |
| 48 | P | 133 | HIS |
| 48 | P | 137 | ASN |
| 49 | p | 33 | GLN |
| 50 | PP | 53 | GLN |
| 50 | PP | 114 | HIS |
| 51 | Q | 44 | ASN |
| 51 | Q | 57 | ASN |
| 51 | Q | 151 | HIS |
| 52 | r | 21 | ASN |
| 52 | r | 70 | GLN |
| 53 | QQ | 48 | GLN |
| 54 | R | 36 | ASN |
| 54 | R | 130 | ASN |
| 54 | R | 141 | HIS |
| 54 | R | 158 | GLN |
| 55 | s | 34 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | s | 200 | ASN |
| 56 | RR | 62 | GLN |
| 56 | RR | 83 | ASN |
| 57 | S | 125 | GLN |
| 58 | t | 100 | HIS |
| 58 | t | 118 | HIS |
| 59 | SS | 19 | ASN |
| 59 | SS | 72 | GLN |
| 59 | SS | 97 | GLN |
| 59 | SS | 120 | HIS |
| 60 | T | 95 | HIS |
| 60 | T | 98 | HIS |
| 61 | TT | 12 | GLN |
| 61 | TT | 63 | HIS |
| 61 | TT | 83 | GLN |
| 61 | TT | 126 | GLN |
| 61 | TT | 137 | GLN |
| 62 | U | 95 | ASN |
| 64 | V | 135 | ASN |
| 68 | WW | 5 | ASN |
| 69 | X | 57 | GLN |
| 71 | XX | 46 | HIS |
| 72 | Y | 14 | ASN |
| 74 | YY | 85 | ASN |
| 74 | YY | 94 | HIS |
| 74 | YY | 112 | ASN |
| 74 | YY | 124 | ASN |
| 75 | Z | 132 | GLN |
| 77 | ZZ | 45 | ASN |
| 77 | ZZ | 64 | ASN |
| 78 | a | 14 | HIS |
| 78 | a | 34 | ASN |
| 78 | a | 40 | HIS |
| 79 | AA | 84 | GLN |
| 79 | AA | 215 | GLN |
| 81 | B | 3 | HIS |
| 81 | B | 275 | HIS |
| 81 | B | 315 | ASN |
| 81 | B | 328 | ASN |
| 82 | c | 15 | ASN |
| 84 | cc | 24 | GLN |
| 84 | cc | 26 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 23 | hh | 14/15 (93%) | 8 (57%) | 0 |
| 67 | 5 | 3516/3705 (94%) | 857 (24%) | 155 (4%) |
| 70 | 7 | 119/120 (99%) | 14 (11%) | 0 |
| 73 | 8 | 149/151 (98%) | 34 (22%) | 5 (3%) |
| 76 | 9 | 1679/1779 (94%) | 420 (25%) | 66 (3%) |
| All | All | 5477/5770 (94%) | 1333 (24%) | 226 (4%) |

All (1333) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | hh | 42 | C |
| 23 | hh | 43 | A |
| 23 | hh | 45 | A |
| 23 | hh | 46 | G |
| 23 | hh | 49 | U |
| 23 | hh | 52 | G |
| 23 | hh | 54 | U |
| 23 | hh | 55 | C |
| 67 | 5 | 12 | A |
| 67 | 5 | 13 | U |
| 67 | 5 | 15 | A |
| 67 | 5 | 25 | A |
| 67 | 5 | 35 | U |
| 67 | 5 | 39 | A |
| 67 | 5 | 42 | A |
| 67 | 5 | 43 | U |
| 67 | 5 | 48 | G |
| 67 | 5 | 49 | U |
| 67 | 5 | 56 | A |
| 67 | 5 | 58 | G |
| 67 | 5 | 59 | A |
| 67 | 5 | 64 | A |
| 67 | 5 | 65 | A |
| 67 | 5 | 73 | A |
| 67 | 5 | 91 | G |
| 67 | 5 | 93 | G |
| 67 | 5 | 109 | G |
| 67 | 5 | 110 | C |
| 67 | 5 | 118 | C |
| 67 | 5 | 119 | G |
| 67 | 5 | 120 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 126 | C |
| 67 | 5 | 134 | G |
| 67 | 5 | 135 | G |
| 67 | 5 | 136 | C |
| 67 | 5 | 137 | G |
| 67 | 5 | 143 | C |
| 67 | 5 | 144 | G |
| 67 | 5 | 159 | C |
| 67 | 5 | 172 | C |
| 67 | 5 | 173 | C |
| 67 | 5 | 177 | G |
| 67 | 5 | 179 | G |
| 67 | 5 | 197 | A |
| 67 | 5 | 200 | U |
| 67 | 5 | 201 | C |
| 67 | 5 | 202 | C |
| 67 | 5 | 205 | C |
| 67 | 5 | 209 | U |
| 67 | 5 | 216 | C |
| 67 | 5 | 218 | A |
| 67 | 5 | 220 | C |
| 67 | 5 | 221 | C |
| 67 | 5 | 224 | U |
| 67 | 5 | 226 | G |
| 67 | 5 | 227 | A |
| 67 | 5 | 233 | U |
| 67 | 5 | 234 | G |
| 67 | 5 | 245 | C |
| 67 | 5 | 246 | G |
| 67 | 5 | 253 | G |
| 67 | 5 | 262 | G |
| 67 | 5 | 263 | G |
| 67 | 5 | 266 | C |
| 67 | 5 | 267 | G |
| 67 | 5 | 276 | C |
| 67 | 5 | 279 | A |
| 67 | 5 | 280 | G |
| 67 | 5 | 281 | U |
| 67 | 5 | 297 | U |
| 67 | 5 | 306 | A |
| 67 | 5 | 309 | C |
| 67 | 5 | 310 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 315 | G |
| 67 | 5 | 316 | U |
| 67 | 5 | 322 | C |
| 67 | 5 | 328 | A |
| 67 | 5 | 334 | A |
| 67 | 5 | 340 | C |
| 67 | 5 | 350 | C |
| 67 | 5 | 357 | U |
| 67 | 5 | 363 | A |
| 67 | 5 | 386 | A |
| 67 | 5 | 387 | G |
| 67 | 5 | 399 | G |
| 67 | 5 | 406 | C |
| 67 | 5 | 407 | A |
| 67 | 5 | 408 | A |
| 67 | 5 | 409 | G |
| 67 | 5 | 410 | A |
| 67 | 5 | 412 | G |
| 67 | 5 | 413 | G |
| 67 | 5 | 414 | C |
| 67 | 5 | 431 | G |
| 67 | 5 | 432 | U |
| 67 | 5 | 446 | C |
| 67 | 5 | 449 | C |
| 67 | 5 | 450 | G |
| 67 | 5 | 452 | A |
| 67 | 5 | 453 | G |
| 67 | 5 | 454 | U |
| 67 | 5 | 457 | G |
| 67 | 5 | 467 | U |
| 67 | 5 | 468 | U |
| 67 | 5 | 469 | C |
| 67 | 5 | 481 | G |
| 67 | 5 | 481(A) | C |
| 67 | 5 | 482 | G |
| 67 | 5 | 483 | G |
| 67 | 5 | 484 | U |
| 67 | 5 | 485 | C |
| 67 | 5 | 486 | C |
| 67 | 5 | 492 | U |
| 67 | 5 | 493 | G |
| 67 | 5 | 495 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 497 | G |
| 67 | 5 | 498 | C |
| 67 | 5 | 499 | G |
| 67 | 5 | 505 | G |
| 67 | 5 | 510 | U |
| 67 | 5 | 649 | A |
| 67 | 5 | 654 | C |
| 67 | 5 | 658 | C |
| 67 | 5 | 666 | G |
| 67 | 5 | 667 | A |
| 67 | 5 | 668 | C |
| 67 | 5 | 672 | C |
| 67 | 5 | 683 | C |
| 67 | 5 | 684 | G |
| 67 | 5 | 685 | C |
| 67 | 5 | 687 | U |
| 67 | 5 | 696 | C |
| 67 | 5 | 697 | G |
| 67 | 5 | 704 | C |
| 67 | 5 | 705 | G |
| 67 | 5 | 708 | G |
| 67 | 5 | 719 | C |
| 67 | 5 | 722 | G |
| 67 | 5 | 729 | G |
| 67 | 5 | 730 | G |
| 67 | 5 | 731 | G |
| 67 | 5 | 734 | G |
| 67 | 5 | 738 | C |
| 67 | 5 | 738(A) | C |
| 67 | 5 | 739 | G |
| 67 | 5 | 747 | A |
| 67 | 5 | 748 | G |
| 67 | 5 | 749 | G |
| 67 | 5 | 750 | U |
| 67 | 5 | 756 | G |
| 67 | 5 | 758 | G |
| 67 | 5 | 911 | U |
| 67 | 5 | 913 | U |
| 67 | 5 | 914 | U |
| 67 | 5 | 916 | C |
| 67 | 5 | 917 | A |
| 67 | 5 | 918 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 923 | C |
| 67 | 5 | 924 | C |
| 67 | 5 | 925 | C |
| 67 | 5 | 926 | G |
| 67 | 5 | 928 | C |
| 67 | 5 | 929 | A |
| 67 | 5 | 931 | C |
| 67 | 5 | 932 | A |
| 67 | 5 | 933 | G |
| 67 | 5 | 934 | C |
| 67 | 5 | 935 | A |
| 67 | 5 | 935(A) | G |
| 67 | 5 | 936 | C |
| 67 | 5 | 938 | C |
| 67 | 5 | 939 | G |
| 67 | 5 | 943 | A |
| 67 | 5 | 944 | A |
| 67 | 5 | 945 | U |
| 67 | 5 | 955 | G |
| 67 | 5 | 956 | A |
| 67 | 5 | 957 | G |
| 67 | 5 | 959 | G |
| 67 | 5 | 960 | A |
| 67 | 5 | 961 | G |
| 67 | 5 | 962 | C |
| 67 | 5 | 965 | G |
| 67 | 5 | 966 | A |
| 67 | 5 | 967 | C |
| 67 | 5 | 968 | C |
| 67 | 5 | 969 | C |
| 67 | 5 | 970 | G |
| 67 | 5 | 972 | C |
| 67 | 5 | 973 | G |
| 67 | 5 | 979 | C |
| 67 | 5 | 983 | C |
| 67 | 5 | 990 | C |
| 67 | 5 | 1072 | C |
| 67 | 5 | 1073 | G |
| 67 | 5 | 1075 | G |
| 67 | 5 | 1076 | C |
| 67 | 5 | 1078 | A |
| 67 | 5 | 1079 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 1082 | C |
| 67 | 5 | 1174 | G |
| 67 | 5 | 1177 | U |
| 67 | 5 | 1179 | U |
| 67 | 5 | 1184 | A |
| 67 | 5 | 1195 | G |
| 67 | 5 | 1211 | G |
| 67 | 5 | 1212 | G |
| 67 | 5 | 1214 | C |
| 67 | 5 | 1215 | C |
| 67 | 5 | 1234 | G |
| 67 | 5 | 1235 | G |
| 67 | 5 | 1236 | C |
| 67 | 5 | 1237 | C |
| 67 | 5 | 1238 | A |
| 67 | 5 | 1239 | C |
| 67 | 5 | 1272 | C |
| 67 | 5 | 1273 | G |
| 67 | 5 | 1274 | A |
| 67 | 5 | 1276 | C |
| 67 | 5 | 1280 | C |
| 67 | 5 | 1284 | G |
| 67 | 5 | 1287 | G |
| 67 | 5 | 1288 | G |
| 67 | 5 | 1291 | G |
| 67 | 5 | 1292 | C |
| 67 | 5 | 1293 | G |
| 67 | 5 | 1295 | U |
| 67 | 5 | 1296 | G |
| 67 | 5 | 1301 | C |
| 67 | 5 | 1303 | A |
| 67 | 5 | 1304 | C |
| 67 | 5 | 1326 | A |
| 67 | 5 | 1328 | G |
| 67 | 5 | 1330 | A |
| 67 | 5 | 1337 | A |
| 67 | 5 | 1354 | A |
| 67 | 5 | 1359 | G |
| 67 | 5 | 1360 | G |
| 67 | 5 | 1364 | U |
| 67 | 5 | 1370 | G |
| 67 | 5 | 1371 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 1377 | G |
| 67 | 5 | 1378 | C |
| 67 | 5 | 1379 | C |
| 67 | 5 | 1380 | G |
| 67 | 5 | 1381 | U |
| 67 | 5 | 1387 | A |
| 67 | 5 | 1394 | G |
| 67 | 5 | 1397 | A |
| 67 | 5 | 1398 | A |
| 67 | 5 | 1401 | C |
| 67 | 5 | 1403 | G |
| 67 | 5 | 1416 | G |
| 67 | 5 | 1418 | C |
| 67 | 5 | 1419 | G |
| 67 | 5 | 1420 | A |
| 67 | 5 | 1421 | G |
| 67 | 5 | 1429 | C |
| 67 | 5 | 1435 | G |
| 67 | 5 | 1436 | C |
| 67 | 5 | 1437 | C |
| 67 | 5 | 1438 | U |
| 67 | 5 | 1441 | C |
| 67 | 5 | 1442 | C |
| 67 | 5 | 1445 | U |
| 67 | 5 | 1446 | C |
| 67 | 5 | 1453 | G |
| 67 | 5 | 1455 | G |
| 67 | 5 | 1456 | C |
| 67 | 5 | 1457 | G |
| 67 | 5 | 1458 | C |
| 67 | 5 | 1465 | G |
| 67 | 5 | 1475 | G |
| 67 | 5 | 1478 | C |
| 67 | 5 | 1481 | C |
| 67 | 5 | 1482 | G |
| 67 | 5 | 1483 | C |
| 67 | 5 | 1484 | G |
| 67 | 5 | 1485 | C |
| 67 | 5 | 1486 | C |
| 67 | 5 | 1489 | G |
| 67 | 5 | 1493 | G |
| 67 | 5 | 1497 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 1498 | G |
| 67 | 5 | 1502 | G |
| 67 | 5 | 1514 | U |
| 67 | 5 | 1516 | G |
| 67 | 5 | 1518 | A |
| 67 | 5 | 1523 | A |
| 67 | 5 | 1525 | A |
| 67 | 5 | 1534 | A |
| 67 | 5 | 1535 | C |
| 67 | 5 | 1547 | A |
| 67 | 5 | 1554 | A |
| 67 | 5 | 1563 | A |
| 67 | 5 | 1564 | A |
| 67 | 5 | 1566 | C |
| 67 | 5 | 1574 | G |
| 67 | 5 | 1578 | U |
| 67 | 5 | 1586 | G |
| 67 | 5 | 1591 | U |
| 67 | 5 | 1596 | U |
| 67 | 5 | 1601 | A |
| 67 | 5 | 1602 | U |
| 67 | 5 | 1612 | G |
| 67 | 5 | 1613 | A |
| 67 | 5 | 1624 | G |
| 67 | 5 | 1625 | G |
| 67 | 5 | 1626 | G |
| 67 | 5 | 1631 | A |
| 67 | 5 | 1633 | G |
| 67 | 5 | 1634 | A |
| 67 | 5 | 1654 | G |
| 67 | 5 | 1656 | U |
| 67 | 5 | 1661 | C |
| 67 | 5 | 1670 | G |
| 67 | 5 | 1676 | C |
| 67 | 5 | 1677 | U |
| 67 | 5 | 1679 | A |
| 67 | 5 | 1691 | G |
| 67 | 5 | 1724 | G |
| 67 | 5 | 1726 | U |
| 67 | 5 | 1734 | G |
| 67 | 5 | 1735 | U |
| 67 | 5 | 1740 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 1741 | G |
| 67 | 5 | 1742 | A |
| 67 | 5 | 1750 | G |
| 67 | 5 | 1753 | G |
| 67 | 5 | 1755 | C |
| 67 | 5 | 1756 | U |
| 67 | 5 | 1757 | U |
| 67 | 5 | 1761 | G |
| 67 | 5 | 1763 | C |
| 67 | 5 | 1764 | G |
| 67 | 5 | 1772 | C |
| 67 | 5 | 1773 | U |
| 67 | 5 | 1776 | A |
| 67 | 5 | 1780 | A |
| 67 | 5 | 1781 | U |
| 67 | 5 | 1787 | A |
| 67 | 5 | 1797 | G |
| 67 | 5 | 1799 | G |
| 67 | 5 | 1800 | U |
| 67 | 5 | 1803 | G |
| 67 | 5 | 1804 | A |
| 67 | 5 | 1805 | A |
| 67 | 5 | 1819 | G |
| 67 | 5 | 1821 | G |
| 67 | 5 | 1822 | U |
| 67 | 5 | 1823 | G |
| 67 | 5 | 1828 | C |
| 67 | 5 | 1833 | G |
| 67 | 5 | 1834 | U |
| 67 | 5 | 1835 | G |
| 67 | 5 | 1836 | G |
| 67 | 5 | 1837 | A |
| 67 | 5 | 1842 | G |
| 67 | 5 | 1855 | G |
| 67 | 5 | 1867 | A |
| 67 | 5 | 1869 | G |
| 67 | 5 | 1882 | U |
| 67 | 5 | 1883 | G |
| 67 | 5 | 1890 | G |
| 67 | 5 | 1893 | C |
| 67 | 5 | 1897 | A |
| 67 | 5 | 1910 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 1918 | U |
| 67 | 5 | 1920 | C |
| 67 | 5 | 1921 | C |
| 67 | 5 | 1922 | G |
| 67 | 5 | 1923 | A |
| 67 | 5 | 1931 | C |
| 67 | 5 | 1933 | G |
| 67 | 5 | 1941 | A |
| 67 | 5 | 1945 | G |
| 67 | 5 | 1948 | G |
| 67 | 5 | 1952 | G |
| 67 | 5 | 1959 | U |
| 67 | 5 | 1961 | G |
| 67 | 5 | 1962 | A |
| 67 | 5 | 1963 | C |
| 67 | 5 | 1966 | C |
| 67 | 5 | 1967 | A |
| 67 | 5 | 1976 | G |
| 67 | 5 | 1977 | C |
| 67 | 5 | 1980 | U |
| 67 | 5 | 1981 | G |
| 67 | 5 | 1982 | G |
| 67 | 5 | 1983 | A |
| 67 | 5 | 1984 | A |
| 67 | 5 | 1986 | U |
| 67 | 5 | 1987 | C |
| 67 | 5 | 1991 | A |
| 67 | 5 | 1997 | U |
| 67 | 5 | 2001 | G |
| 67 | 5 | 2002 | A |
| 67 | 5 | 2003 | G |
| 67 | 5 | 2004 | U |
| 67 | 5 | 2005 | G |
| 67 | 5 | 2008 | U |
| 67 | 5 | 2011 | C |
| 67 | 5 | 2024 | G |
| 67 | 5 | 2025 | A |
| 67 | 5 | 2026 | A |
| 67 | 5 | 2046 | G |
| 67 | 5 | 2047 | A |
| 67 | 5 | 2048 | U |
| 67 | 5 | 2052 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 2055 | G |
| 67 | 5 | 2056 | G |
| 67 | 5 | 2062 | C |
| 67 | 5 | 2064 | G |
| 67 | 5 | 2069 | A |
| 67 | 5 | 2070 | U |
| 67 | 5 | 2084 | U |
| 67 | 5 | 2085 | G |
| 67 | 5 | 2089 | G |
| 67 | 5 | 2090 | U |
| 67 | 5 | 2092 | G |
| 67 | 5 | 2093 | G |
| 67 | 5 | 2094 | C |
| 67 | 5 | 2095 | A |
| 67 | 5 | 2097 | A |
| 67 | 5 | 2098 | G |
| 67 | 5 | 2100 | G |
| 67 | 5 | 2101 | A |
| 67 | 5 | 2102 | G |
| 67 | 5 | 2104 | A |
| 67 | 5 | 2106 | G |
| 67 | 5 | 2107 | A |
| 67 | 5 | 2108 | G |
| 67 | 5 | 2110 | G |
| 67 | 5 | 2259 | G |
| 67 | 5 | 2260 | C |
| 67 | 5 | 2262 | G |
| 67 | 5 | 2266 | C |
| 67 | 5 | 2267 | U |
| 67 | 5 | 2268 | A |
| 67 | 5 | 2269 | C |
| 67 | 5 | 2270 | G |
| 67 | 5 | 2275 | G |
| 67 | 5 | 2278 | G |
| 67 | 5 | 2279 | A |
| 67 | 5 | 2288 | G |
| 67 | 5 | 2289 | C |
| 67 | 5 | 2295 | C |
| 67 | 5 | 2300 | A |
| 67 | 5 | 2301 | G |
| 67 | 5 | 2313 | A |
| 67 | 5 | 2314 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 2322 | G |
| 67 | 5 | 2331 | G |
| 67 | 5 | 2333 | G |
| 67 | 5 | 2348 | G |
| 67 | 5 | 2351 | C |
| 67 | 5 | 2364 | G |
| 67 | 5 | 2370 | A |
| 67 | 5 | 2395 | A |
| 67 | 5 | 2396 | A |
| 67 | 5 | 2399 | G |
| 67 | 5 | 2402 | G |
| 67 | 5 | 2416 | G |
| 67 | 5 | 2417 | A |
| 67 | 5 | 2422 | C |
| 67 | 5 | 2424 | G |
| 67 | 5 | 2425 | U |
| 67 | 5 | 2428 | A |
| 67 | 5 | 2429 | A |
| 67 | 5 | 2433 | G |
| 67 | 5 | 2441 | C |
| 67 | 5 | 2450 | G |
| 67 | 5 | 2469 | C |
| 67 | 5 | 2470 | C |
| 67 | 5 | 2471 | G |
| 67 | 5 | 2475 | G |
| 67 | 5 | 2479 | G |
| 67 | 5 | 2483 | G |
| 67 | 5 | 2485 | U |
| 67 | 5 | 2488 | C |
| 67 | 5 | 2489 | C |
| 67 | 5 | 2490 | U |
| 67 | 5 | 2491 | C |
| 67 | 5 | 2493 | G |
| 67 | 5 | 2495 | U |
| 67 | 5 | 2503 | G |
| 67 | 5 | 2504 | C |
| 67 | 5 | 2505 | C |
| 67 | 5 | 2506 | G |
| 67 | 5 | 2511 | A |
| 67 | 5 | 2513 | A |
| 67 | 5 | 2521 | G |
| 67 | 5 | 2530 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 2537 | A |
| 67 | 5 | 2546 | G |
| 67 | 5 | 2547 | G |
| 67 | 5 | 2554 | U |
| 67 | 5 | 2555 | G |
| 67 | 5 | 2564 | G |
| 67 | 5 | 2566 | G |
| 67 | 5 | 2571 | C |
| 67 | 5 | 2572 | C |
| 67 | 5 | 2575 | U |
| 67 | 5 | 2583 | C |
| 67 | 5 | 2586 | G |
| 67 | 5 | 2587 | A |
| 67 | 5 | 2601 | A |
| 67 | 5 | 2618 | G |
| 67 | 5 | 2620 | G |
| 67 | 5 | 2627 | C |
| 67 | 5 | 2638 | G |
| 67 | 5 | 2640 | G |
| 67 | 5 | 2647 | A |
| 67 | 5 | 2661 | U |
| 67 | 5 | 2662 | G |
| 67 | 5 | 2663 | G |
| 67 | 5 | 2669 | C |
| 67 | 5 | 2670 | C |
| 67 | 5 | 2673 | G |
| 67 | 5 | 2676 | A |
| 67 | 5 | 2681 | G |
| 67 | 5 | 2686 | G |
| 67 | 5 | 2687 | U |
| 67 | 5 | 2688 | G |
| 67 | 5 | 2689 | C |
| 67 | 5 | 2695 | A |
| 67 | 5 | 2696 | A |
| 67 | 5 | 2707 | U |
| 67 | 5 | 2708 | U |
| 67 | 5 | 2709 | C |
| 67 | 5 | 2710 | C |
| 67 | 5 | 2711 | G |
| 67 | 5 | 2712 | G |
| 67 | 5 | 2714 | G |
| 67 | 5 | 2716 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 2719 | C |
| 67 | 5 | 2721 | G |
| 67 | 5 | 2725 | A |
| 67 | 5 | 2726 | G |
| 67 | 5 | 2740 | U |
| 67 | 5 | 2743 | A |
| 67 | 5 | 2744 | A |
| 67 | 5 | 2754 | G |
| 67 | 5 | 2760 | G |
| 67 | 5 | 2761 | U |
| 67 | 5 | 2763 | U |
| 67 | 5 | 2764 | A |
| 67 | 5 | 2769 | U |
| 67 | 5 | 2772 | C |
| 67 | 5 | 2787 | A |
| 67 | 5 | 2788 | U |
| 67 | 5 | 2789 | A |
| 67 | 5 | 2790 | U |
| 67 | 5 | 2794 | C |
| 67 | 5 | 2795 | A |
| 67 | 5 | 2796 | G |
| 67 | 5 | 2798 | A |
| 67 | 5 | 2806 | A |
| 67 | 5 | 2807 | A |
| 67 | 5 | 2808 | G |
| 67 | 5 | 2814 | C |
| 67 | 5 | 2826 | U |
| 67 | 5 | 2827 | G |
| 67 | 5 | 2828 | U |
| 67 | 5 | 2829 | U |
| 67 | 5 | 2835 | A |
| 67 | 5 | 2838 | G |
| 67 | 5 | 2839 | U |
| 67 | 5 | 2842 | G |
| 67 | 5 | 2845 | A |
| 67 | 5 | 2855 | G |
| 67 | 5 | 2864 | A |
| 67 | 5 | 2875 | C |
| 67 | 5 | 2884 | G |
| 67 | 5 | 2896 | G |
| 67 | 5 | 2897 | G |
| 67 | 5 | 3598 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 3599 | A |
| 67 | 5 | 3604 | A |
| 67 | 5 | 3605 | C |
| 67 | 5 | 3615 | G |
| 67 | 5 | 3625 | G |
| 67 | 5 | 3626 | G |
| 67 | 5 | 3635 | A |
| 67 | 5 | 3644 | U |
| 67 | 5 | 3653 | A |
| 67 | 5 | 3662 | A |
| 67 | 5 | 3671 | G |
| 67 | 5 | 3673 | C |
| 67 | 5 | 3674 | G |
| 67 | 5 | 3692 | A |
| 67 | 5 | 3696 | C |
| 67 | 5 | 3698 | G |
| 67 | 5 | 3711 | A |
| 67 | 5 | 3712 | A |
| 67 | 5 | 3722 | G |
| 67 | 5 | 3729 | U |
| 67 | 5 | 3740 | G |
| 67 | 5 | 3748 | A |
| 67 | 5 | 3750 | G |
| 67 | 5 | 3753 | G |
| 67 | 5 | 3756 | A |
| 67 | 5 | 3759 | A |
| 67 | 5 | 3760 | A |
| 67 | 5 | 3765 | G |
| 67 | 5 | 3766 | A |
| 67 | 5 | 3773 | U |
| 67 | 5 | 3774 | A |
| 67 | 5 | 3776 | G |
| 67 | 5 | 3777 | G |
| 67 | 5 | 3778 | U |
| 67 | 5 | 3783 | A |
| 67 | 5 | 3784 | A |
| 67 | 5 | 3785 | A |
| 67 | 5 | 3786 | U |
| 67 | 5 | 3799 | A |
| 67 | 5 | 3810 | C |
| 67 | 5 | 3811 | G |
| 67 | 5 | 3812 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 3814 | U |
| 67 | 5 | 3817 | A |
| 67 | 5 | 3819 | G |
| 67 | 5 | 3822 | U |
| 67 | 5 | 3831 | U |
| 67 | 5 | 3838 | U |
| 67 | 5 | 3840 | U |
| 67 | 5 | 3851 | U |
| 67 | 5 | 3859 | G |
| 67 | 5 | 3867 | A |
| 67 | 5 | 3876 | A |
| 67 | 5 | 3877 | A |
| 67 | 5 | 3878 | C |
| 67 | 5 | 3879 | G |
| 67 | 5 | 3889 | G |
| 67 | 5 | 3892 | U |
| 67 | 5 | 3897 | G |
| 67 | 5 | 3898 | G |
| 67 | 5 | 3901 | A |
| 67 | 5 | 3905 | A |
| 67 | 5 | 3906 | A |
| 67 | 5 | 3907 | G |
| 67 | 5 | 3915 | U |
| 67 | 5 | 3916 | G |
| 67 | 5 | 3917 | A |
| 67 | 5 | 3927 | U |
| 67 | 5 | 3939 | G |
| 67 | 5 | 3943 | A |
| 67 | 5 | 3946 | G |
| 67 | 5 | 4067 | U |
| 67 | 5 | 4069 | U |
| 67 | 5 | 4071 | U |
| 67 | 5 | 4076 | G |
| 67 | 5 | 4084 | G |
| 67 | 5 | 4085 | A |
| 67 | 5 | 4086 | G |
| 67 | 5 | 4088 | C |
| 67 | 5 | 4099 | G |
| 67 | 5 | 4100 | C |
| 67 | 5 | 4116 | C |
| 67 | 5 | 4117 | U |
| 67 | 5 | 4118 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 4119 | C |
| 67 | 5 | 4120 | U |
| 67 | 5 | 4121 | G |
| 67 | 5 | 4122 | G |
| 67 | 5 | 4125 | C |
| 67 | 5 | 4127 | A |
| 67 | 5 | 4150 | G |
| 67 | 5 | 4158 | C |
| 67 | 5 | 4162 | C |
| 67 | 5 | 4163 | U |
| 67 | 5 | 4164 | C |
| 67 | 5 | 4166 | G |
| 67 | 5 | 4171 | C |
| 67 | 5 | 4183 | G |
| 67 | 5 | 4184 | G |
| 67 | 5 | 4190 | U |
| 67 | 5 | 4191 | G |
| 67 | 5 | 4203 | A |
| 67 | 5 | 4212 | A |
| 67 | 5 | 4213 | A |
| 67 | 5 | 4218 | U |
| 67 | 5 | 4219 | A |
| 67 | 5 | 4225 | G |
| 67 | 5 | 4229 | U |
| 67 | 5 | 4232 | U |
| 67 | 5 | 4233 | A |
| 67 | 5 | 4249 | G |
| 67 | 5 | 4251 | A |
| 67 | 5 | 4255 | A |
| 67 | 5 | 4257 | A |
| 67 | 5 | 4258 | C |
| 67 | 5 | 4265 | U |
| 67 | 5 | 4268 | A |
| 67 | 5 | 4271 | A |
| 67 | 5 | 4273 | A |
| 67 | 5 | 4281 | A |
| 67 | 5 | 4291 | G |
| 67 | 5 | 4297 | G |
| 67 | 5 | 4304 | A |
| 67 | 5 | 4305 | G |
| 67 | 5 | 4306 | U |
| 67 | 5 | 4314 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 4317 | A |
| 67 | 5 | 4318 | C |
| 67 | 5 | 4319 | C |
| 67 | 5 | 4326 | G |
| 67 | 5 | 4329 | G |
| 67 | 5 | 4330 | G |
| 67 | 5 | 4335 | C |
| 67 | 5 | 4336 | A |
| 67 | 5 | 4339 | A |
| 67 | 5 | 4349 | C |
| 67 | 5 | 4350 | C |
| 67 | 5 | 4354 | U |
| 67 | 5 | 4355 | G |
| 67 | 5 | 4373 | G |
| 67 | 5 | 4377 | G |
| 67 | 5 | 4378 | A |
| 67 | 5 | 4379 | A |
| 67 | 5 | 4380 | A |
| 67 | 5 | 4387 | C |
| 67 | 5 | 4391 | G |
| 67 | 5 | 4393 | G |
| 67 | 5 | 4394 | A |
| 67 | 5 | 4395 | U |
| 67 | 5 | 4396 | A |
| 67 | 5 | 4398 | C |
| 67 | 5 | 4401 | G |
| 67 | 5 | 4415 | A |
| 67 | 5 | 4419 | U |
| 67 | 5 | 4421 | C |
| 67 | 5 | 4422 | A |
| 67 | 5 | 4440 | G |
| 67 | 5 | 4444 | C |
| 67 | 5 | 4448 | G |
| 67 | 5 | 4449 | A |
| 67 | 5 | 4450 | U |
| 67 | 5 | 4453 | C |
| 67 | 5 | 4464 | A |
| 67 | 5 | 4471 | U |
| 67 | 5 | 4475 | G |
| 67 | 5 | 4476 | C |
| 67 | 5 | 4488 | A |
| 67 | 5 | 4495 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 4500 | U |
| 67 | 5 | 4510 | A |
| 67 | 5 | 4511 | A |
| 67 | 5 | 4512 | U |
| 67 | 5 | 4513 | A |
| 67 | 5 | 4519 | C |
| 67 | 5 | 4520 | G |
| 67 | 5 | 4524 | G |
| 67 | 5 | 4531 | U |
| 67 | 5 | 4548 | A |
| 67 | 5 | 4549 | G |
| 67 | 5 | 4560 | C |
| 67 | 5 | 4567 | G |
| 67 | 5 | 4570 | G |
| 67 | 5 | 4573 | G |
| 67 | 5 | 4575 | G |
| 67 | 5 | 4578 | G |
| 67 | 5 | 4586 | G |
| 67 | 5 | 4590 | A |
| 67 | 5 | 4618 | G |
| 67 | 5 | 4627 | U |
| 67 | 5 | 4636 | U |
| 67 | 5 | 4637 | G |
| 67 | 5 | 4639 | G |
| 67 | 5 | 4656 | A |
| 67 | 5 | 4657 | U |
| 67 | 5 | 4661 | G |
| 67 | 5 | 4667 | C |
| 67 | 5 | 4670 | C |
| 67 | 5 | 4672 | A |
| 67 | 5 | 4677 | U |
| 67 | 5 | 4678 | G |
| 67 | 5 | 4687 | A |
| 67 | 5 | 4694 | G |
| 67 | 5 | 4700 | A |
| 67 | 5 | 4701 | A |
| 67 | 5 | 4709 | U |
| 67 | 5 | 4719 | G |
| 67 | 5 | 4720 | C |
| 67 | 5 | 4721 | G |
| 67 | 5 | 4728 | U |
| 67 | 5 | 4736 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 4737 | G |
| 67 | 5 | 4745 | G |
| 67 | 5 | 4751 | G |
| 67 | 5 | 4754 | G |
| 67 | 5 | 4755 | G |
| 67 | 5 | 4756 | C |
| 67 | 5 | 4757 | C |
| 67 | 5 | 4759 | C |
| 67 | 5 | 4761 | G |
| 67 | 5 | 4765 | G |
| 67 | 5 | 4771 | C |
| 67 | 5 | 4772 | C |
| 67 | 5 | 4868 | G |
| 67 | 5 | 4870 | G |
| 67 | 5 | 4871 | C |
| 67 | 5 | 4872 | G |
| 67 | 5 | 4873 | G |
| 67 | 5 | 4874 | A |
| 67 | 5 | 4875 | G |
| 67 | 5 | 4876 | A |
| 67 | 5 | 4877 | G |
| 67 | 5 | 4882 | U |
| 67 | 5 | 4883 | C |
| 67 | 5 | 4885 | U |
| 67 | 5 | 4887 | C |
| 67 | 5 | 4891 | G |
| 67 | 5 | 4895 | C |
| 67 | 5 | 4897 | G |
| 67 | 5 | 4910 | A |
| 67 | 5 | 4912 | G |
| 67 | 5 | 4914 | G |
| 67 | 5 | 4915 | G |
| 67 | 5 | 4918 | C |
| 67 | 5 | 4919 | G |
| 67 | 5 | 4921 | C |
| 67 | 5 | 4924 | C |
| 67 | 5 | 4925 | U |
| 67 | 5 | 4926 | C |
| 67 | 5 | 4928 | C |
| 67 | 5 | 4931 | G |
| 67 | 5 | 4935 | C |
| 67 | 5 | 4937 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 4938 | A |
| 67 | 5 | 4940 | C |
| 67 | 5 | 4943 | A |
| 67 | 5 | 4944 | C |
| 67 | 5 | 4948 | C |
| 67 | 5 | 4949 | G |
| 67 | 5 | 4950 | U |
| 67 | 5 | 4951 | G |
| 67 | 5 | 4956 | A |
| 67 | 5 | 4957 | C |
| 67 | 5 | 4958 | C |
| 67 | 5 | 4964 | C |
| 67 | 5 | 4965 | U |
| 67 | 5 | 4966 | A |
| 67 | 5 | 4967 | A |
| 67 | 5 | 4976 | U |
| 67 | 5 | 4985 | U |
| 67 | 5 | 4988 | U |
| 67 | 5 | 4989 | U |
| 67 | 5 | 4990 | C |
| 67 | 5 | 4991 | U |
| 67 | 5 | 4993 | G |
| 67 | 5 | 5007 | A |
| 67 | 5 | 5014 | A |
| 67 | 5 | 5017 | G |
| 67 | 5 | 5035 | U |
| 67 | 5 | 5040 | U |
| 67 | 5 | 5041 | G |
| 67 | 5 | 5047 | C |
| 67 | 5 | 5050 | C |
| 67 | 5 | 5052 | C |
| 67 | 5 | 5053 | U |
| 67 | 5 | 5054 | C |
| 67 | 5 | 5056 | A |
| 67 | 5 | 5061 | A |
| 67 | 5 | 5062 | G |
| 70 | 7 | 7 | G |
| 70 | 7 | 11 | A |
| 70 | 7 | 22 | A |
| 70 | 7 | 25 | G |
| 70 | 7 | 33 | U |
| 70 | 7 | 42 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 70 | 7 | 53 | U |
| 70 | 7 | 54 | A |
| 70 | 7 | 64 | G |
| 70 | 7 | 97 | G |
| 70 | 7 | 100 | A |
| 70 | 7 | 106 | G |
| 70 | 7 | 110 | G |
| 70 | 7 | 120 | U |
| 73 | 8 | 2 | G |
| 73 | 8 | 3 | A |
| 73 | 8 | 32 | C |
| 73 | 8 | 34 | U |
| 73 | 8 | 35 | C |
| 73 | 8 | 49 | G |
| 73 | 8 | 59 | A |
| 73 | 8 | 62 | A |
| 73 | 8 | 63 | U |
| 73 | 8 | 75 | G |
| 73 | 8 | 79 | G |
| 73 | 8 | 86 | U |
| 73 | 8 | 87 | G |
| 73 | 8 | 94 | G |
| 73 | 8 | 95 | A |
| 73 | 8 | 103 | A |
| 73 | 8 | 104 | A |
| 73 | 8 | 105 | C |
| 73 | 8 | 107 | C |
| 73 | 8 | 109 | C |
| 73 | 8 | 110 | U |
| 73 | 8 | 111 | U |
| 73 | 8 | 112 | G |
| 73 | 8 | 114 | G |
| 73 | 8 | 121 | G |
| 73 | 8 | 123 | U |
| 73 | 8 | 124 | U |
| 73 | 8 | 125 | C |
| 73 | 8 | 126 | C |
| 73 | 8 | 127 | U |
| 73 | 8 | 137 | A |
| 73 | 8 | 143 | G |
| 73 | 8 | 150 | C |
| 73 | 8 | 153 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 2 | A |
| 76 | 9 | 3 | C |
| 76 | 9 | 4 | C |
| 76 | 9 | 17 | C |
| 76 | 9 | 25 | A |
| 76 | 9 | 26 | U |
| 76 | 9 | 33 | G |
| 76 | 9 | 41 | G |
| 76 | 9 | 44 | U |
| 76 | 9 | 45 | A |
| 76 | 9 | 46 | A |
| 76 | 9 | 56 | G |
| 76 | 9 | 58 | C |
| 76 | 9 | 60 | A |
| 76 | 9 | 65 | C |
| 76 | 9 | 67 | C |
| 76 | 9 | 68 | A |
| 76 | 9 | 70 | G |
| 76 | 9 | 71 | G |
| 76 | 9 | 73 | C |
| 76 | 9 | 74 | G |
| 76 | 9 | 75 | G |
| 76 | 9 | 77 | A |
| 76 | 9 | 79 | A |
| 76 | 9 | 99 | A |
| 76 | 9 | 100 | U |
| 76 | 9 | 103 | A |
| 76 | 9 | 104 | A |
| 76 | 9 | 110 | U |
| 76 | 9 | 111 | A |
| 76 | 9 | 113 | G |
| 76 | 9 | 115 | U |
| 76 | 9 | 116 | U |
| 76 | 9 | 124 | U |
| 76 | 9 | 126 | G |
| 76 | 9 | 127 | C |
| 76 | 9 | 129 | C |
| 76 | 9 | 130 | G |
| 76 | 9 | 141 | A |
| 76 | 9 | 143 | U |
| 76 | 9 | 147 | A |
| 76 | 9 | 155 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 158 | A |
| 76 | 9 | 161 | U |
| 76 | 9 | 162 | C |
| 76 | 9 | 163 | U |
| 76 | 9 | 167 | G |
| 76 | 9 | 168 | C |
| 76 | 9 | 173 | A |
| 76 | 9 | 175 | A |
| 76 | 9 | 182 | C |
| 76 | 9 | 183 | G |
| 76 | 9 | 184 | G |
| 76 | 9 | 188 | C |
| 76 | 9 | 189 | U |
| 76 | 9 | 192 | C |
| 76 | 9 | 200 | G |
| 76 | 9 | 202 | G |
| 76 | 9 | 206 | G |
| 76 | 9 | 213 | G |
| 76 | 9 | 215 | G |
| 76 | 9 | 289 | G |
| 76 | 9 | 292 | A |
| 76 | 9 | 293 | C |
| 76 | 9 | 294 | U |
| 76 | 9 | 302 | A |
| 76 | 9 | 304 | C |
| 76 | 9 | 307 | G |
| 76 | 9 | 308 | G |
| 76 | 9 | 309 | G |
| 76 | 9 | 312 | G |
| 76 | 9 | 314 | U |
| 76 | 9 | 318 | A |
| 76 | 9 | 319 | C |
| 76 | 9 | 322 | C |
| 76 | 9 | 331 | C |
| 76 | 9 | 332 | G |
| 76 | 9 | 335 | G |
| 76 | 9 | 340 | C |
| 76 | 9 | 347 | G |
| 76 | 9 | 351 | G |
| 76 | 9 | 360 | A |
| 76 | 9 | 362 | C |
| 76 | 9 | 364 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 368 | U |
| 76 | 9 | 370 | G |
| 76 | 9 | 371 | A |
| 76 | 9 | 372 | U |
| 76 | 9 | 381 | C |
| 76 | 9 | 382 | C |
| 76 | 9 | 383 | G |
| 76 | 9 | 384 | U |
| 76 | 9 | 385 | G |
| 76 | 9 | 386 | C |
| 76 | 9 | 400 | C |
| 76 | 9 | 407 | G |
| 76 | 9 | 409 | C |
| 76 | 9 | 417 | C |
| 76 | 9 | 418 | A |
| 76 | 9 | 435 | A |
| 76 | 9 | 438 | G |
| 76 | 9 | 448 | A |
| 76 | 9 | 449 | A |
| 76 | 9 | 450 | C |
| 76 | 9 | 459 | C |
| 76 | 9 | 460 | A |
| 76 | 9 | 462 | C |
| 76 | 9 | 464 | A |
| 76 | 9 | 465 | A |
| 76 | 9 | 466 | G |
| 76 | 9 | 472 | C |
| 76 | 9 | 473 | A |
| 76 | 9 | 474 | G |
| 76 | 9 | 476 | A |
| 76 | 9 | 482 | G |
| 76 | 9 | 487 | U |
| 76 | 9 | 492 | C |
| 76 | 9 | 496 | C |
| 76 | 9 | 507 | G |
| 76 | 9 | 508 | A |
| 76 | 9 | 512 | A |
| 76 | 9 | 516 | A |
| 76 | 9 | 525 | A |
| 76 | 9 | 531 | A |
| 76 | 9 | 532 | C |
| 76 | 9 | 533 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 544 | G |
| 76 | 9 | 545 | A |
| 76 | 9 | 546 | G |
| 76 | 9 | 548 | C |
| 76 | 9 | 549 | C |
| 76 | 9 | 550 | C |
| 76 | 9 | 551 | U |
| 76 | 9 | 554 | A |
| 76 | 9 | 555 | A |
| 76 | 9 | 556 | U |
| 76 | 9 | 557 | U |
| 76 | 9 | 559 | G |
| 76 | 9 | 563 | G |
| 76 | 9 | 564 | A |
| 76 | 9 | 568 | C |
| 76 | 9 | 576 | A |
| 76 | 9 | 583 | A |
| 76 | 9 | 587 | A |
| 76 | 9 | 588 | G |
| 76 | 9 | 589 | G |
| 76 | 9 | 590 | A |
| 76 | 9 | 591 | U |
| 76 | 9 | 592 | C |
| 76 | 9 | 597 | G |
| 76 | 9 | 598 | G |
| 76 | 9 | 604 | A |
| 76 | 9 | 606 | G |
| 76 | 9 | 607 | U |
| 76 | 9 | 608 | C |
| 76 | 9 | 614 | C |
| 76 | 9 | 620 | G |
| 76 | 9 | 629 | A |
| 76 | 9 | 631 | U |
| 76 | 9 | 637 | U |
| 76 | 9 | 643 | A |
| 76 | 9 | 644 | G |
| 76 | 9 | 655 | A |
| 76 | 9 | 659 | G |
| 76 | 9 | 660 | C |
| 76 | 9 | 663 | C |
| 76 | 9 | 664 | A |
| 76 | 9 | 668 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 669 | A |
| 76 | 9 | 670 | A |
| 76 | 9 | 671 | A |
| 76 | 9 | 672 | A |
| 76 | 9 | 673 | G |
| 76 | 9 | 684 | G |
| 76 | 9 | 688 | U |
| 76 | 9 | 689 | U |
| 76 | 9 | 732 | U |
| 76 | 9 | 752 | G |
| 76 | 9 | 753 | C |
| 76 | 9 | 754 | G |
| 76 | 9 | 810 | A |
| 76 | 9 | 811 | A |
| 76 | 9 | 812 | A |
| 76 | 9 | 821 | G |
| 76 | 9 | 822 | U |
| 76 | 9 | 830 | A |
| 76 | 9 | 834 | C |
| 76 | 9 | 847 | A |
| 76 | 9 | 861 | A |
| 76 | 9 | 868 | G |
| 76 | 9 | 869 | A |
| 76 | 9 | 870 | A |
| 76 | 9 | 871 | U |
| 76 | 9 | 872 | A |
| 76 | 9 | 873 | G |
| 76 | 9 | 874 | G |
| 76 | 9 | 875 | A |
| 76 | 9 | 877 | C |
| 76 | 9 | 878 | G |
| 76 | 9 | 885 | U |
| 76 | 9 | 887 | U |
| 76 | 9 | 890 | U |
| 76 | 9 | 892 | U |
| 76 | 9 | 913 | A |
| 76 | 9 | 914 | U |
| 76 | 9 | 920 | A |
| 76 | 9 | 922 | A |
| 76 | 9 | 930 | C |
| 76 | 9 | 933 | G |
| 76 | 9 | 934 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 943 | U |
| 76 | 9 | 955 | A |
| 76 | 9 | 971 | G |
| 76 | 9 | 985 | G |
| 76 | 9 | 990 | A |
| 76 | 9 | 992 | A |
| 76 | 9 | 999 | G |
| 76 | 9 | 1008 | A |
| 76 | 9 | 1017 | U |
| 76 | 9 | 1023 | A |
| 76 | 9 | 1041 | G |
| 76 | 9 | 1045 | U |
| 76 | 9 | 1060 | A |
| 76 | 9 | 1061 | U |
| 76 | 9 | 1062 | A |
| 76 | 9 | 1078 | C |
| 76 | 9 | 1083 | A |
| 76 | 9 | 1085 | C |
| 76 | 9 | 1089 | G |
| 76 | 9 | 1096 | G |
| 76 | 9 | 1099 | G |
| 76 | 9 | 1100 | A |
| 76 | 9 | 1113 | A |
| 76 | 9 | 1114 | U |
| 76 | 9 | 1115 | U |
| 76 | 9 | 1116 | C |
| 76 | 9 | 1117 | C |
| 76 | 9 | 1118 | C |
| 76 | 9 | 1121 | G |
| 76 | 9 | 1131 | G |
| 76 | 9 | 1133 | A |
| 76 | 9 | 1138 | C |
| 76 | 9 | 1139 | C |
| 76 | 9 | 1148 | A |
| 76 | 9 | 1149 | A |
| 76 | 9 | 1150 | A |
| 76 | 9 | 1153 | C |
| 76 | 9 | 1154 | U |
| 76 | 9 | 1165 | G |
| 76 | 9 | 1166 | G |
| 76 | 9 | 1195 | A |
| 76 | 9 | 1197 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 1207 | G |
| 76 | 9 | 1208 | A |
| 76 | 9 | 1211 | G |
| 76 | 9 | 1213 | C |
| 76 | 9 | 1215 | C |
| 76 | 9 | 1216 | C |
| 76 | 9 | 1221 | G |
| 76 | 9 | 1223 | A |
| 76 | 9 | 1224 | G |
| 76 | 9 | 1240 | A |
| 76 | 9 | 1242 | U |
| 76 | 9 | 1251 | A |
| 76 | 9 | 1253 | A |
| 76 | 9 | 1254 | C |
| 76 | 9 | 1256 | G |
| 76 | 9 | 1257 | G |
| 76 | 9 | 1259 | A |
| 76 | 9 | 1260 | A |
| 76 | 9 | 1265 | A |
| 76 | 9 | 1271 | C |
| 76 | 9 | 1274 | G |
| 76 | 9 | 1275 | G |
| 76 | 9 | 1281 | G |
| 76 | 9 | 1284 | A |
| 76 | 9 | 1285 | G |
| 76 | 9 | 1286 | G |
| 76 | 9 | 1287 | A |
| 76 | 9 | 1289 | U |
| 76 | 9 | 1293 | A |
| 76 | 9 | 1298 | G |
| 76 | 9 | 1299 | A |
| 76 | 9 | 1300 | U |
| 76 | 9 | 1301 | A |
| 76 | 9 | 1302 | G |
| 76 | 9 | 1307 | U |
| 76 | 9 | 1308 | U |
| 76 | 9 | 1313 | A |
| 76 | 9 | 1314 | U |
| 76 | 9 | 1316 | C |
| 76 | 9 | 1330 | G |
| 76 | 9 | 1331 | C |
| 76 | 9 | 1342 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 1348 | G |
| 76 | 9 | 1354 | G |
| 76 | 9 | 1369 | A |
| 76 | 9 | 1371 | U |
| 76 | 9 | 1372 | U |
| 76 | 9 | 1378 | A |
| 76 | 9 | 1395 | C |
| 76 | 9 | 1396 | A |
| 76 | 9 | 1397 | U |
| 76 | 9 | 1401 | A |
| 76 | 9 | 1402 | A |
| 76 | 9 | 1404 | U |
| 76 | 9 | 1410 | C |
| 76 | 9 | 1412 | C |
| 76 | 9 | 1424 | G |
| 76 | 9 | 1428 | G |
| 76 | 9 | 1429 | G |
| 76 | 9 | 1439 | A |
| 76 | 9 | 1449 | G |
| 76 | 9 | 1452 | A |
| 76 | 9 | 1454 | A |
| 76 | 9 | 1458 | G |
| 76 | 9 | 1459 | G |
| 76 | 9 | 1462 | U |
| 76 | 9 | 1463 | U |
| 76 | 9 | 1466 | G |
| 76 | 9 | 1473 | G |
| 76 | 9 | 1476 | A |
| 76 | 9 | 1477 | U |
| 76 | 9 | 1478 | U |
| 76 | 9 | 1490 | G |
| 76 | 9 | 1494 | U |
| 76 | 9 | 1495 | G |
| 76 | 9 | 1497 | G |
| 76 | 9 | 1498 | A |
| 76 | 9 | 1507 | G |
| 76 | 9 | 1509 | U |
| 76 | 9 | 1510 | G |
| 76 | 9 | 1519 | U |
| 76 | 9 | 1520 | G |
| 76 | 9 | 1521 | C |
| 76 | 9 | 1522 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 1531 | A |
| 76 | 9 | 1533 | A |
| 76 | 9 | 1536 | G |
| 76 | 9 | 1544 | C |
| 76 | 9 | 1545 | A |
| 76 | 9 | 1548 | G |
| 76 | 9 | 1552 | G |
| 76 | 9 | 1553 | C |
| 76 | 9 | 1555 | U |
| 76 | 9 | 1556 | A |
| 76 | 9 | 1557 | C |
| 76 | 9 | 1560 | U |
| 76 | 9 | 1570 | G |
| 76 | 9 | 1574 | C |
| 76 | 9 | 1575 | G |
| 76 | 9 | 1580 | A |
| 76 | 9 | 1581 | C |
| 76 | 9 | 1582 | C |
| 76 | 9 | 1585 | U |
| 76 | 9 | 1586 | U |
| 76 | 9 | 1587 | G |
| 76 | 9 | 1588 | A |
| 76 | 9 | 1589 | A |
| 76 | 9 | 1600 | G |
| 76 | 9 | 1601 | A |
| 76 | 9 | 1602 | U |
| 76 | 9 | 1604 | G |
| 76 | 9 | 1621 | U |
| 76 | 9 | 1623 | A |
| 76 | 9 | 1625 | U |
| 76 | 9 | 1637 | A |
| 76 | 9 | 1638 | G |
| 76 | 9 | 1639 | G |
| 76 | 9 | 1641 | A |
| 76 | 9 | 1647 | A |
| 76 | 9 | 1648 | G |
| 76 | 9 | 1654 | G |
| 76 | 9 | 1664 | A |
| 76 | 9 | 1665 | G |
| 76 | 9 | 1671 | G |
| 76 | 9 | 1680 | G |
| 76 | 9 | 1682 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 1683 | C |
| 76 | 9 | 1686 | G |
| 76 | 9 | 1689 | C |
| 76 | 9 | 1695 | A |
| 76 | 9 | 1698 | C |
| 76 | 9 | 1699 | A |
| 76 | 9 | 1700 | C |
| 76 | 9 | 1703 | C |
| 76 | 9 | 1715 | A |
| 76 | 9 | 1721 | U |
| 76 | 9 | 1722 | G |
| 76 | 9 | 1726 | G |
| 76 | 9 | 1728 | U |
| 76 | 9 | 1729 | U |
| 76 | 9 | 1730 | U |
| 76 | 9 | 1737 | G |
| 76 | 9 | 1753 | C |
| 76 | 9 | 1756 | C |
| 76 | 9 | 1758 | G |
| 76 | 9 | 1760 | G |
| 76 | 9 | 1772 | C |
| 76 | 9 | 1783 | C |
| 76 | 9 | 1785 | C |
| 76 | 9 | 1800 | A |
| 76 | 9 | 1823 | A |
| 76 | 9 | 1825 | A |
| 76 | 9 | 1826 | G |
| 76 | 9 | 1829 | G |
| 76 | 9 | 1831 | A |
| 76 | 9 | 1835 | A |
| 76 | 9 | 1836 | G |
| 76 | 9 | 1838 | U |
| 76 | 9 | 1849 | G |
| 76 | 9 | 1851 | A |
| 76 | 9 | 1861 | G |
| 76 | 9 | 1862 | G |
| 76 | 9 | 1863 | A |
| 76 | 9 | 1865 | C |
| 76 | 9 | 1866 | A |
| 76 | 9 | 1867 | U |
| 76 | 9 | 1868 | U |
| 76 | 9 | 1869 | A |

All (226) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 12 | A |
| 67 | 5 | 47 | A |
| 67 | 5 | 48 | G |
| 67 | 5 | 64 | A |
| 67 | 5 | 119 | G |
| 67 | 5 | 125 | C |
| 67 | 5 | 134 | G |
| 67 | 5 | 143 | C |
| 67 | 5 | 159 | C |
| 67 | 5 | 217 | C |
| 67 | 5 | 226 | G |
| 67 | 5 | 234 | G |
| 67 | 5 | 245 | C |
| 67 | 5 | 265 | C |
| 67 | 5 | 275 | C |
| 67 | 5 | 278 | G |
| 67 | 5 | 385 | A |
| 67 | 5 | 387 | G |
| 67 | 5 | 406 | C |
| 67 | 5 | 408 | A |
| 67 | 5 | 409 | G |
| 67 | 5 | 449 | C |
| 67 | 5 | 480 | C |
| 67 | 5 | 481(A) | C |
| 67 | 5 | 482 | G |
| 67 | 5 | 484 | U |
| 67 | 5 | 485 | C |
| 67 | 5 | 492 | U |
| 67 | 5 | 497 | G |
| 67 | 5 | 498 | C |
| 67 | 5 | 504 | G |
| 67 | 5 | 696 | C |
| 67 | 5 | 729 | G |
| 67 | 5 | 738(A) | C |
| 67 | 5 | 747 | A |
| 67 | 5 | 748 | G |
| 67 | 5 | 915 | A |
| 67 | 5 | 916 | C |
| 67 | 5 | 930 | G |
| 67 | 5 | 935(A) | G |
| 67 | 5 | 955 | G |
| 67 | 5 | 956 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 959 | G |
| 67 | 5 | 965 | G |
| 67 | 5 | 966 | A |
| 67 | 5 | 969 | C |
| 67 | 5 | 971(A) | G |
| 67 | 5 | 1071 | C |
| 67 | 5 | 1072 | C |
| 67 | 5 | 1211 | G |
| 67 | 5 | 1214 | C |
| 67 | 5 | 1236 | C |
| 67 | 5 | 1238 | A |
| 67 | 5 | 1287 | G |
| 67 | 5 | 1291 | G |
| 67 | 5 | 1295 | U |
| 67 | 5 | 1329 | G |
| 67 | 5 | 1354 | A |
| 67 | 5 | 1358 | G |
| 67 | 5 | 1359 | G |
| 67 | 5 | 1370 | G |
| 67 | 5 | 1378 | C |
| 67 | 5 | 1380 | G |
| 67 | 5 | 1420 | A |
| 67 | 5 | 1440 | U |
| 67 | 5 | 1445 | U |
| 67 | 5 | 1455 | G |
| 67 | 5 | 1477 | C |
| 67 | 5 | 1481 | C |
| 67 | 5 | 1484 | G |
| 67 | 5 | 1485 | C |
| 67 | 5 | 1497 | A |
| 67 | 5 | 1502 | G |
| 67 | 5 | 1563 | A |
| 67 | 5 | 1633 | G |
| 67 | 5 | 1733 | G |
| 67 | 5 | 1734 | G |
| 67 | 5 | 1740 | C |
| 67 | 5 | 1804 | A |
| 67 | 5 | 1815 | G |
| 67 | 5 | 1818 | G |
| 67 | 5 | 1833 | G |
| 67 | 5 | 1834 | U |
| 67 | 5 | 1835 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 1836 | G |
| 67 | 5 | 1881 | C |
| 67 | 5 | 1892 | A |
| 67 | 5 | 1921 | C |
| 67 | 5 | 1935 | C |
| 67 | 5 | 1979 | A |
| 67 | 5 | 1983 | A |
| 67 | 5 | 2046 | G |
| 67 | 5 | 2068 | C |
| 67 | 5 | 2088 | A |
| 67 | 5 | 2089 | G |
| 67 | 5 | 2100 | G |
| 67 | 5 | 2265 | G |
| 67 | 5 | 2266 | C |
| 67 | 5 | 2278 | G |
| 67 | 5 | 2313 | A |
| 67 | 5 | 2398 | U |
| 67 | 5 | 2428 | A |
| 67 | 5 | 2467 | U |
| 67 | 5 | 2468 | U |
| 67 | 5 | 2474 | G |
| 67 | 5 | 2475 | G |
| 67 | 5 | 2490 | U |
| 67 | 5 | 2502 | A |
| 67 | 5 | 2546 | G |
| 67 | 5 | 2587 | A |
| 67 | 5 | 2661 | U |
| 67 | 5 | 2695 | A |
| 67 | 5 | 2754 | G |
| 67 | 5 | 2794 | C |
| 67 | 5 | 2806 | A |
| 67 | 5 | 3625 | G |
| 67 | 5 | 3673 | C |
| 67 | 5 | 3697 | U |
| 67 | 5 | 3710 | G |
| 67 | 5 | 3765 | G |
| 67 | 5 | 3809 | G |
| 67 | 5 | 3876 | A |
| 67 | 5 | 3888 | G |
| 67 | 5 | 3904 | G |
| 67 | 5 | 4075 | U |
| 67 | 5 | 4076 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | 5 | 4084 | G |
| 67 | 5 | 4119 | C |
| 67 | 5 | 4121 | G |
| 67 | 5 | 4124 | G |
| 67 | 5 | 4162 | C |
| 67 | 5 | 4170 | A |
| 67 | 5 | 4232 | U |
| 67 | 5 | 4254 | G |
| 67 | 5 | 4266 | G |
| 67 | 5 | 4378 | A |
| 67 | 5 | 4395 | U |
| 67 | 5 | 4448 | G |
| 67 | 5 | 4449 | A |
| 67 | 5 | 4510 | A |
| 67 | 5 | 4527 | G |
| 67 | 5 | 4626 | A |
| 67 | 5 | 4694 | G |
| 67 | 5 | 4699 | U |
| 67 | 5 | 4719 | G |
| 67 | 5 | 4871 | C |
| 67 | 5 | 4872 | G |
| 67 | 5 | 4876 | A |
| 67 | 5 | 4884 | G |
| 67 | 5 | 4925 | U |
| 67 | 5 | 4936 | G |
| 67 | 5 | 4942 | C |
| 67 | 5 | 4947 | U |
| 67 | 5 | 4965 | U |
| 67 | 5 | 4966 | A |
| 73 | 8 | 2 | G |
| 73 | 8 | 86 | U |
| 73 | 8 | 94 | G |
| 73 | 8 | 110 | U |
| 73 | 8 | 124 | U |
| 76 | 9 | 2 | A |
| 76 | 9 | 72 | C |
| 76 | 9 | 110 | U |
| 76 | 9 | 126 | G |
| 76 | 9 | 160 | U |
| 76 | 9 | 182 | C |
| 76 | 9 | 293 | C |
| 76 | 9 | 308 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 369 | C |
| 76 | 9 | 370 | G |
| 76 | 9 | 434 | G |
| 76 | 9 | 448 | A |
| 76 | 9 | 465 | A |
| 76 | 9 | 473 | A |
| 76 | 9 | 487 | U |
| 76 | 9 | 532 | C |
| 76 | 9 | 550 | C |
| 76 | 9 | 553 | U |
| 76 | 9 | 555 | A |
| 76 | 9 | 563 | G |
| 76 | 9 | 591 | U |
| 76 | 9 | 606 | G |
| 76 | 9 | 620 | G |
| 76 | 9 | 642 | U |
| 76 | 9 | 670 | A |
| 76 | 9 | 688 | U |
| 76 | 9 | 752 | G |
| 76 | 9 | 821 | G |
| 76 | 9 | 869 | A |
| 76 | 9 | 870 | A |
| 76 | 9 | 872 | A |
| 76 | 9 | 874 | G |
| 76 | 9 | 1016 | U |
| 76 | 9 | 1114 | U |
| 76 | 9 | 1115 | U |
| 76 | 9 | 1120 | U |
| 76 | 9 | 1137 | U |
| 76 | 9 | 1165 | G |
| 76 | 9 | 1215 | C |
| 76 | 9 | 1253 | A |
| 76 | 9 | 1264 | C |
| 76 | 9 | 1284 | A |
| 76 | 9 | 1286 | G |
| 76 | 9 | 1313 | A |
| 76 | 9 | 1330 | G |
| 76 | 9 | 1394 | G |
| 76 | 9 | 1395 | C |
| 76 | 9 | 1396 | A |
| 76 | 9 | 1489 | A |
| 76 | 9 | 1493 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 76 | 9 | 1519 | U |
| 76 | 9 | 1520 | G |
| 76 | 9 | 1535 | U |
| 76 | 9 | 1585 | U |
| 76 | 9 | 1637 | A |
| 76 | 9 | 1638 | G |
| 76 | 9 | 1646 | C |
| 76 | 9 | 1664 | A |
| 76 | 9 | 1665 | G |
| 76 | 9 | 1679 | A |
| 76 | 9 | 1721 | U |
| 76 | 9 | 1744 | G |
| 76 | 9 | 1824 | A |
| 76 | 9 | 1835 | A |
| 76 | 9 | 1867 | U |
| 76 | 9 | 1868 | U |

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 291 ligands modelled in this entry, 289 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 87 | GCP | jj | 700 | - | 27,34,34 | 4.66 | 10 (37%) | 34,54,54 | 1.74 | 8 (23%) |
| 88 | BLS | 5 | 5122 | 67 | 28,31,31 | 3.73 | 14 (50%) | 28,43,43 | 2.06 | 10 (35%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 87 | GCP | jj | 700 | - | - | 5/15/38/38 | 0/3/3/3 |
| 88 | BLS | 5 | 5122 | 67 | - | 8/21/38/38 | 0/2/2/2 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 87 | jj | 700 | GCP | O4'-C1' | 15.21 | 1.62 | 1.41 |
| 87 | jj | 700 | GCP | C2'-C1' | -14.43 | 1.31 | 1.53 |
| 88 | 5 | 5122 | BLS | O5'-C5' | -11.48 | 1.24 | 1.43 |
| 88 | 5 | 5122 | BLS | C3'-C2' | 7.36 | 1.55 | 1.33 |
| 88 | 5 | 5122 | BLS | C4'-C5' | 7.17 | 1.69 | 1.53 |
| 87 | jj | 700 | GCP | O4'-C4' | -6.12 | 1.31 | 1.45 |
| 87 | jj | 700 | GCP | PB-O3A | 5.67 | 1.64 | 1.58 |
| 88 | 5 | 5122 | BLS | C7-N6 | 5.45 | 1.45 | 1.34 |
| 87 | jj | 700 | GCP | C2-N2 | 5.28 | 1.44 | 1.33 |
| 88 | 5 | 5122 | BLS | C14-N12 | 4.76 | 1.45 | 1.35 |
| 88 | 5 | 5122 | BLS | C14-N15 | 4.52 | 1.44 | 1.34 |
| 88 | 5 | 5122 | BLS | C1'-C2' | -3.91 | 1.40 | 1.49 |
| 88 | 5 | 5122 | BLS | C4-N4 | 3.52 | 1.45 | 1.35 |
| 87 | jj | 700 | GCP | O3'-C3' | -3.05 | 1.35 | 1.43 |
| 87 | jj | 700 | GCP | O2'-C2' | 2.88 | 1.49 | 1.43 |
| 88 | 5 | 5122 | BLS | C1'-N1 | -2.75 | 1.41 | 1.49 |
| 87 | jj | 700 | GCP | C5-C4 | -2.68 | 1.33 | 1.40 |
| 88 | 5 | 5122 | BLS | C4'-C3' | -2.52 | 1.40 | 1.49 |
| 88 | 5 | 5122 | BLS | C5-C4 | -2.48 | 1.35 | 1.41 |
| 88 | 5 | 5122 | BLS | O7-C7 | -2.45 | 1.18 | 1.23 |
| 88 | 5 | 5122 | BLS | C6-N1 | -2.42 | 1.32 | 1.35 |
| 87 | jj | 700 | GCP | PB-O2B | -2.33 | 1.50 | 1.56 |
| 88 | 5 | 5122 | BLS | C5'-C6' | 2.27 | 1.57 | 1.53 |
| 87 | jj | 700 | GCP | O6-C6 | -2.08 | 1.19 | 1.24 |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 88 | 5 | 5122 | BLS | C8-C7-N6 | 4.97 | 122.84 | 116.33 |
| 87 | jj | 700 | GCP | N3-C2-N1 | -4.76 | 120.88 | 127.22 |
| 87 | jj | 700 | GCP | C2-N3-C4 | 4.62 | 120.63 | 115.36 |
| 88 | 5 | 5122 | BLS | C4-N3-C2 | 3.71 | 120.10 | 116.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 87 | jj | 700 | GCP | PB-O3A-PA | -3.32 | 122.04 | 132.56 |
| 88 | 5 | 5122 | BLS | C11-C10-C9 | -3.21 | 108.49 | 114.52 |
| 88 | 5 | 5122 | BLS | C4'-N6-C7 | -3.15 | 119.76 | 123.13 |
| 88 | 5 | 5122 | BLS | O5'-C1'-C2' | -3.09 | 111.46 | 113.13 |
| 88 | 5 | 5122 | BLS | N4-C4-N3 | 3.06 | 121.33 | 116.49 |
| 88 | 5 | 5122 | BLS | O7-C7-C8 | -2.93 | 117.21 | 121.50 |
| 87 | jj | 700 | GCP | C5-C6-N1 | -2.61 | 119.86 | 123.43 |
| 87 | jj | 700 | GCP | C4-C5-N7 | -2.55 | 106.74 | 109.40 |
| 87 | jj | 700 | GCP | N2-C2-N1 | 2.51 | 121.15 | 117.25 |
| 87 | jj | 700 | GCP | C2'-C3'-C4' | -2.46 | 97.86 | 102.64 |
| 87 | jj | 700 | GCP | C3'-C2'-C1' | 2.42 | 104.61 | 100.98 |
| 88 | 5 | 5122 | BLS | C1'-C2'-C3' | -2.35 | 119.44 | 122.52 |
| 88 | 5 | 5122 | BLS | O4-C6'-O3 | -2.15 | 119.20 | 124.09 |
| 88 | 5 | 5122 | BLS | C3'-C4'-N6 | -2.12 | 106.70 | 110.60 |

There are no chirality outliers.

All (13) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 87 | jj | 700 | GCP | PG-C3B-PB-O1B |
| 87 | jj | 700 | GCP | PG-C3B-PB-O2B |
| 87 | jj | 700 | GCP | PG-C3B-PB-O3A |
| 87 | jj | 700 | GCP | C5'-O5'-PA-O3A |
| 88 | 5 | 5122 | BLS | C3'-C4'-N6-C7 |
| 88 | 5 | 5122 | BLS | C7-C8-C9-N9 |
| 88 | 5 | 5122 | BLS | C11-C10-C9-C8 |
| 88 | 5 | 5122 | BLS | C11-C10-C9-N9 |
| 88 | 5 | 5122 | BLS | N6-C7-C8-C9 |
| 88 | 5 | 5122 | BLS | O7-C7-C8-C9 |
| 87 | jj | 700 | GCP | C5'-O5'-PA-O2A |
| 88 | 5 | 5122 | BLS | C7-C8-C9-C10 |
| 88 | 5 | 5122 | BLS | C5'-C4'-N6-C7 |

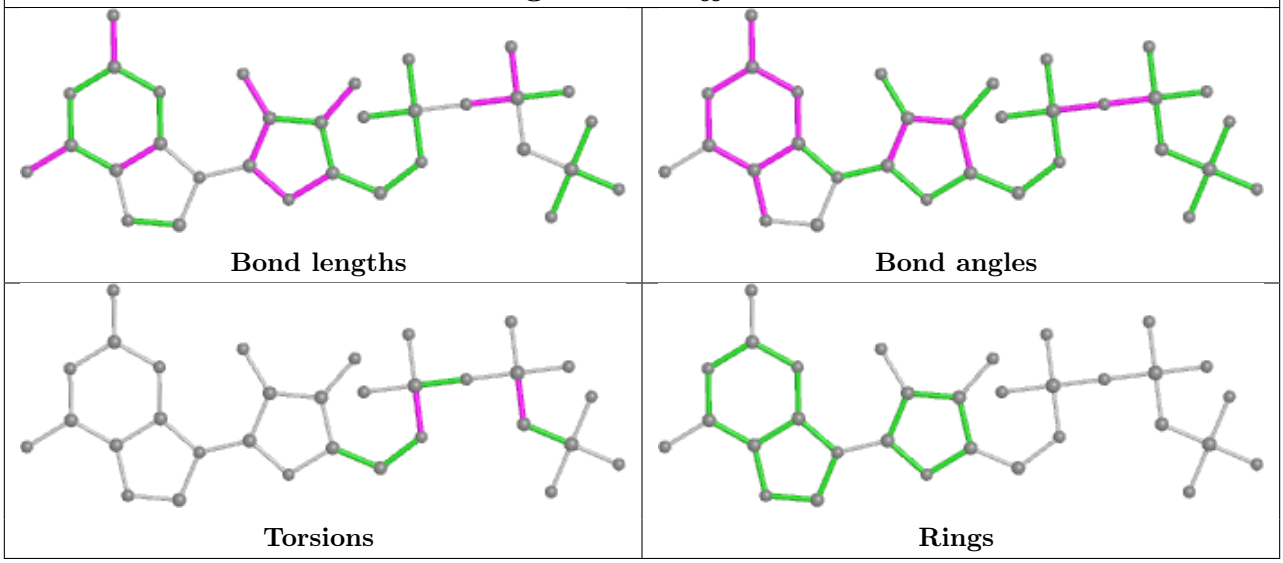
There are no ring outliers.

No monomer is involved in short contacts.

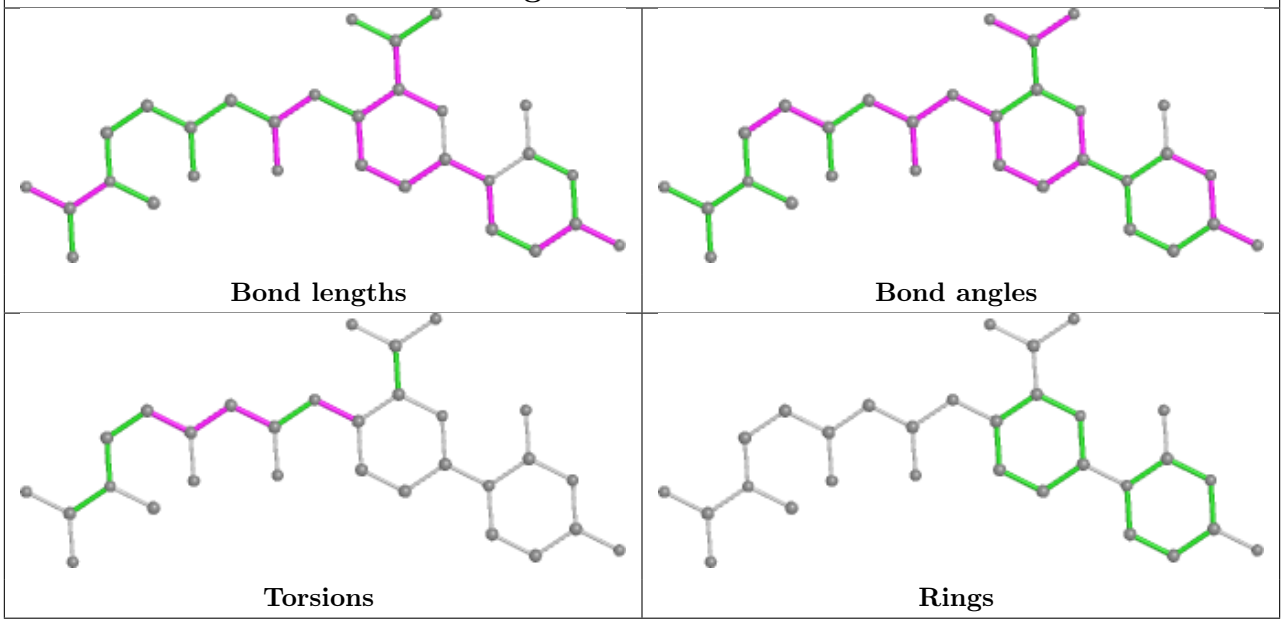
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand GCP jj 700**




**Ligand BLS 5 5122**




## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 67 | 5 | 7 |
| 76 | 9 | 7 |
| 73 | 8 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | 5 | 990:C | O3' | 1064:G | P | 17.61 |
| 1 | 5 | 1406(C):G | O3' | 1411:C | P | 17.48 |
| 1 | 8 | 79:G | O3' | 85:U | P | 15.70 |
| 1 | 5 | 4138:C | O3' | 4146:G | P | 15.08 |
| 1 | 9 | 322:C | O3' | 323:C | P | 9.57 |
| 1 | 9 | 798:G | O3' | 799:U | P | 5.28 |
| 1 | 5 | 1438:U | O3' | 1440:U | P | 4.98 |
| 1 | 9 | 1295:A | O3' | 1296:U | P | 4.76 |
| 1 | 5 | 5020:G | O3' | 5021:C | P | 4.72 |
| 1 | 9 | 304:C | O3' | 305:U | P | 4.39 |
| 1 | 5 | 170:C | O3' | 171:U | P | 4.32 |
| 1 | 5 | 751:G | O3' | 752:G | P | 3.76 |
| 1 | 9 | 902:G | O3' | 903:A | P | 3.75 |
| 1 | 9 | 309:G | O3' | 310:C | P | 3.57 |
| 1 | 9 | 903:A | O3' | 904:A | P | 3.28 |

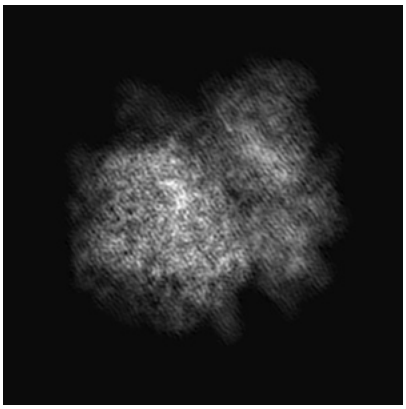
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12632. These allow visual inspection of the internal detail of the map and identification of artifacts.

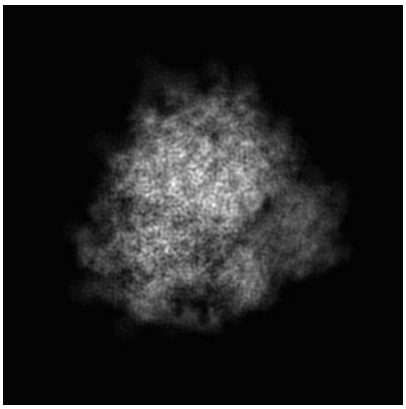
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

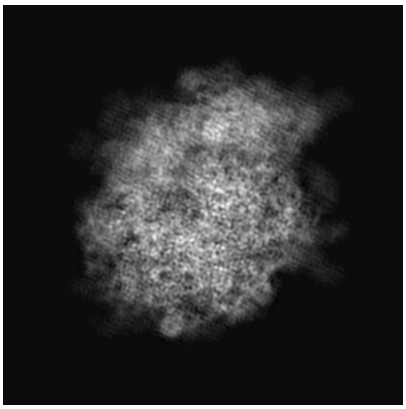
### 6.1.1 Primary map



X

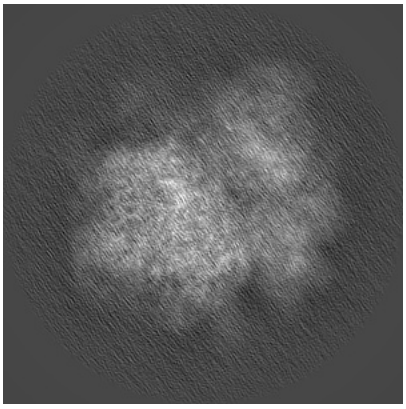


Y

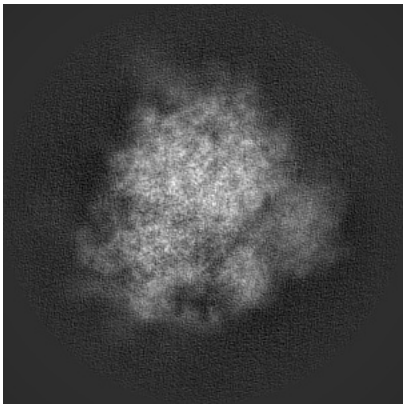


Z

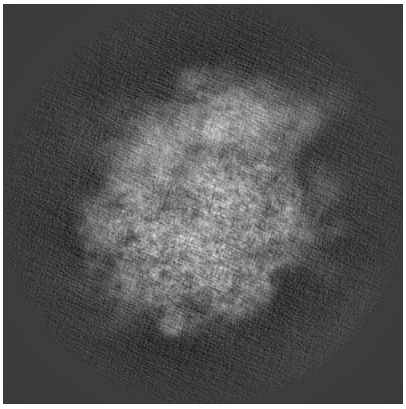
### 6.1.2 Raw map



X



Y

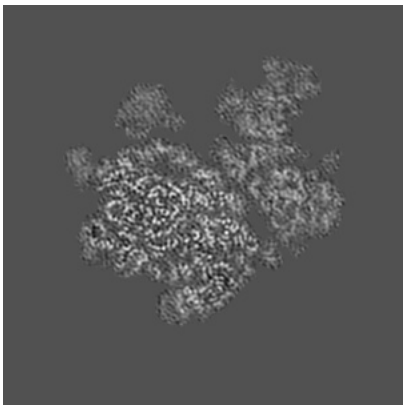


Z

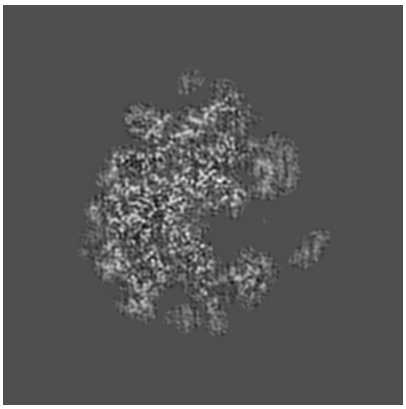
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

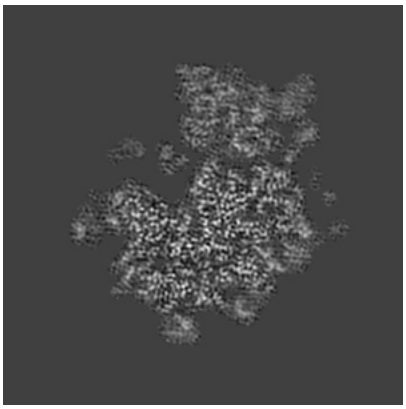
### 6.2.1 Primary map



X Index: 150

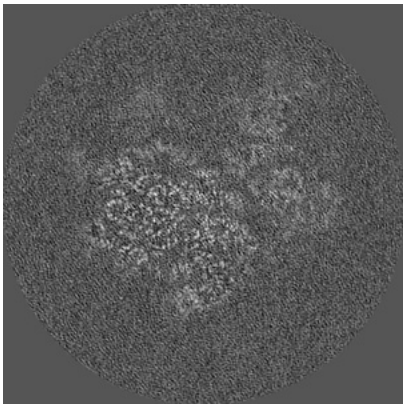


Y Index: 150

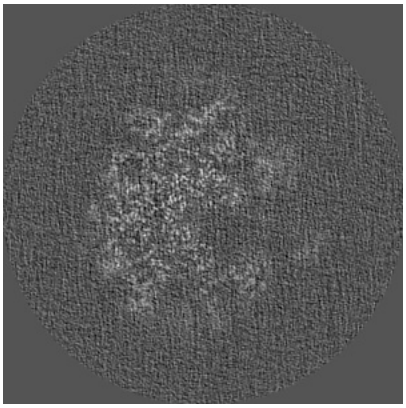


Z Index: 150

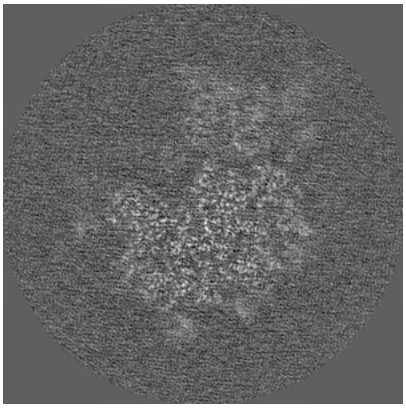
### 6.2.2 Raw map



X Index: 150



Y Index: 150

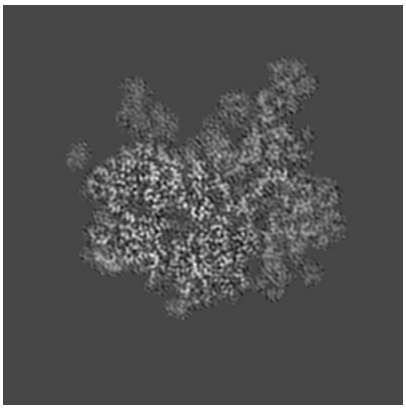


Z Index: 150

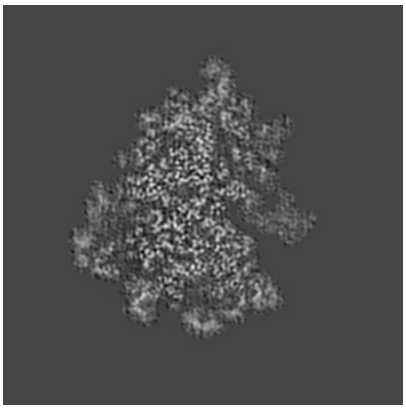
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

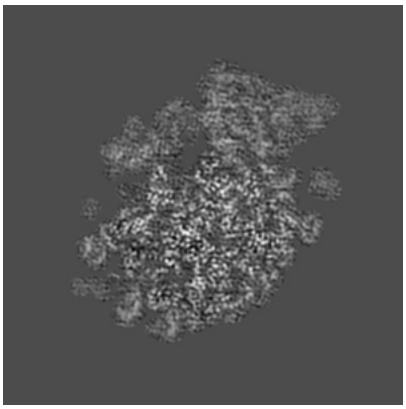
### 6.3.1 Primary map



X Index: 158

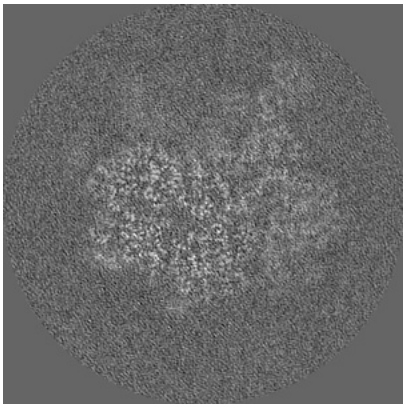


Y Index: 130

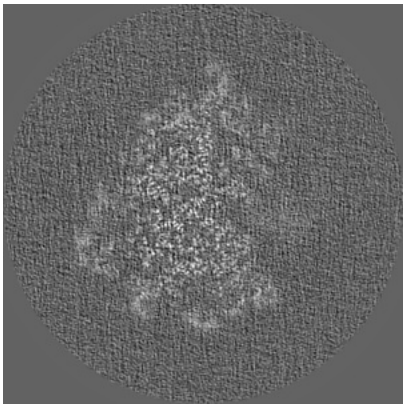


Z Index: 128

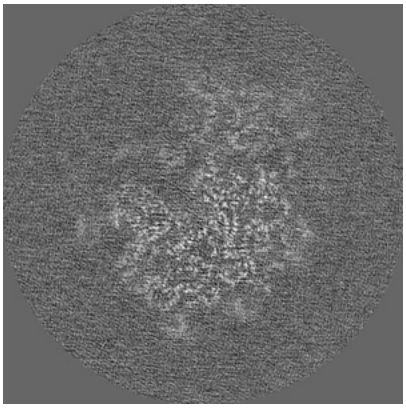
### 6.3.2 Raw map



X Index: 158



Y Index: 130

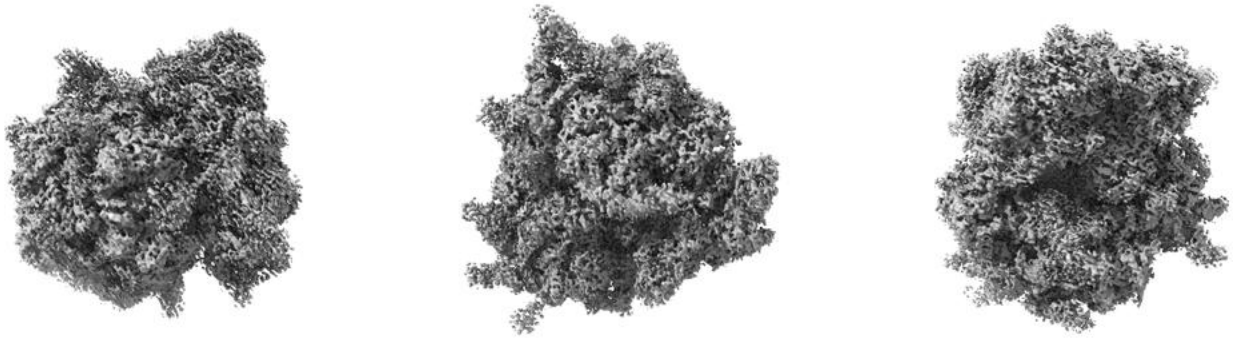


Z Index: 148

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

## 6.4 Orthogonal surface views (i)

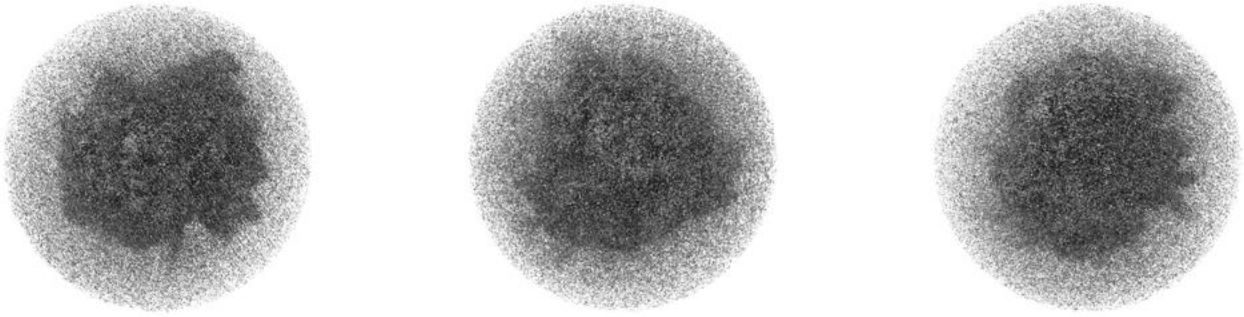
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

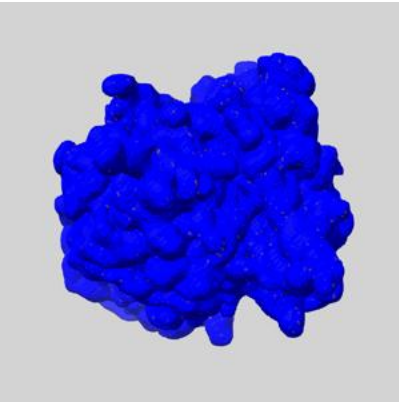
## 6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

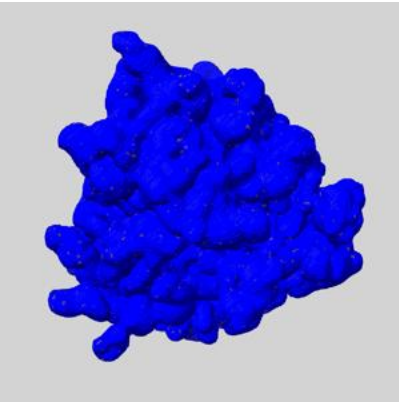
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

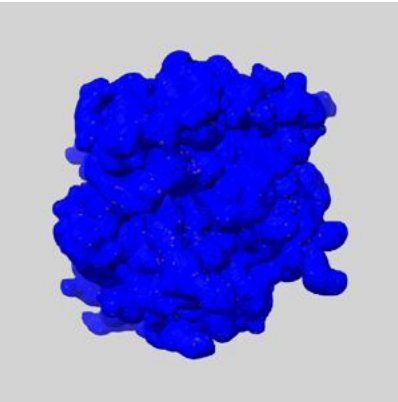
### 6.5.1 emd_12632_msk_1.map (i)



X



Y

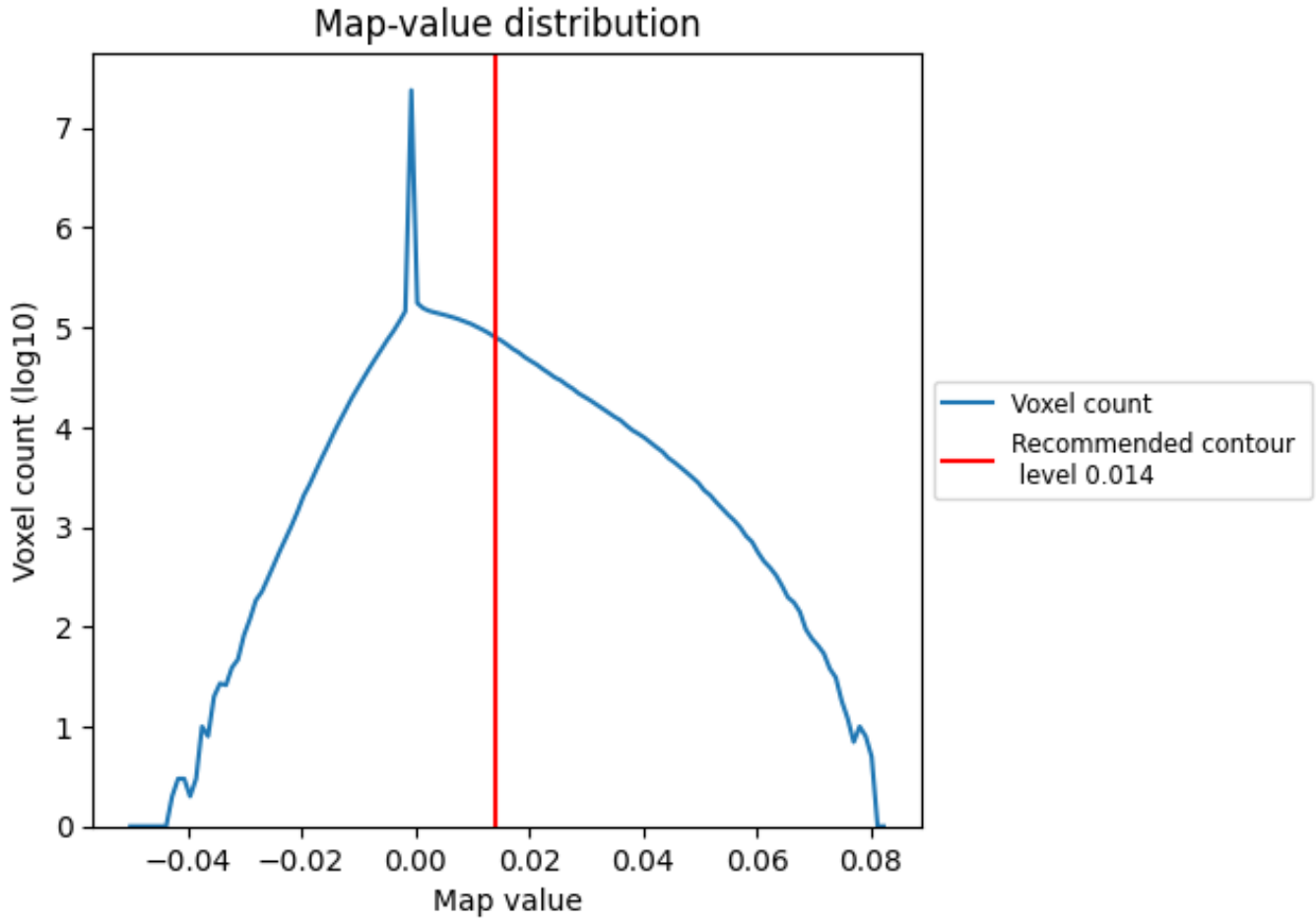


Z

# 7 Map analysis

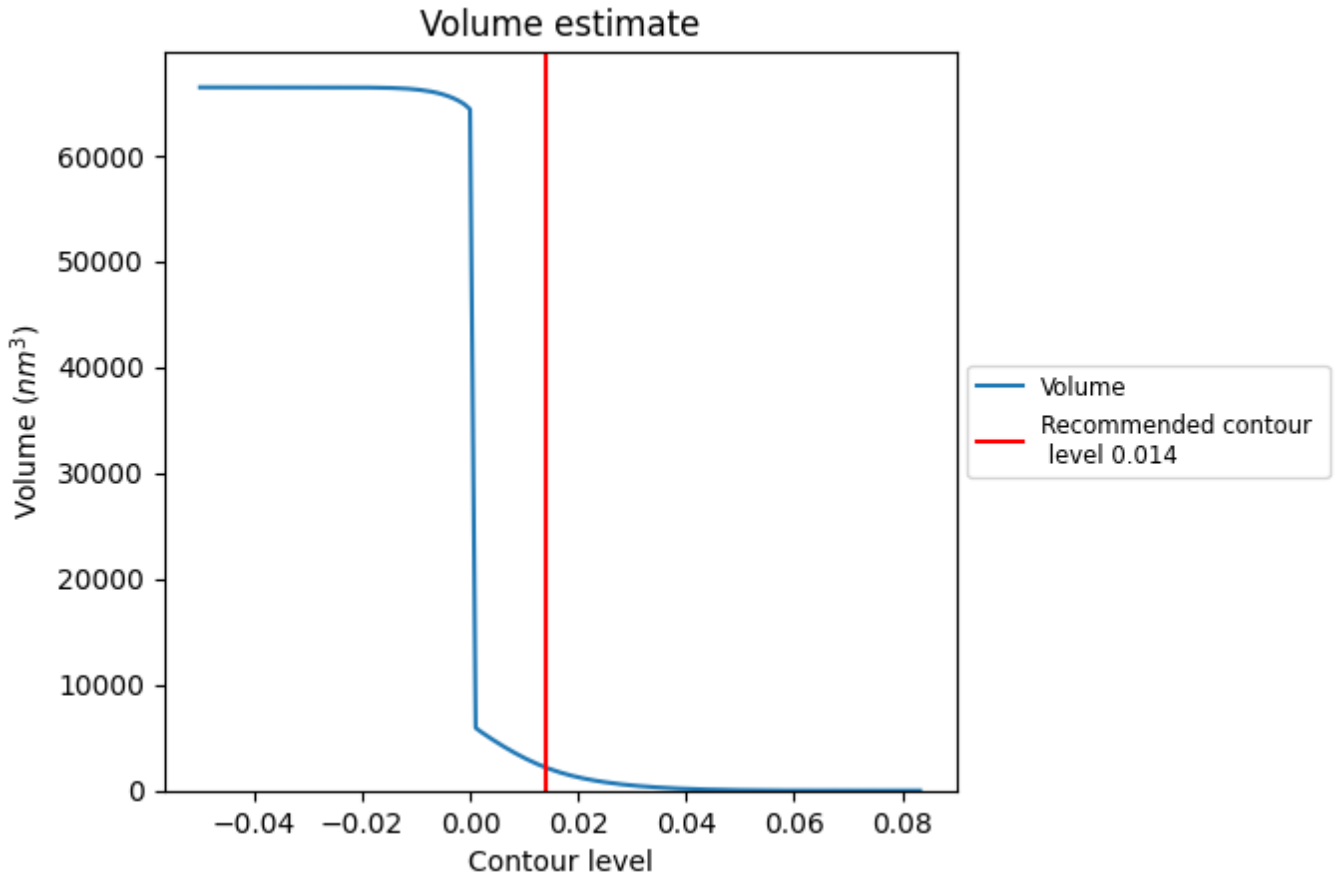
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

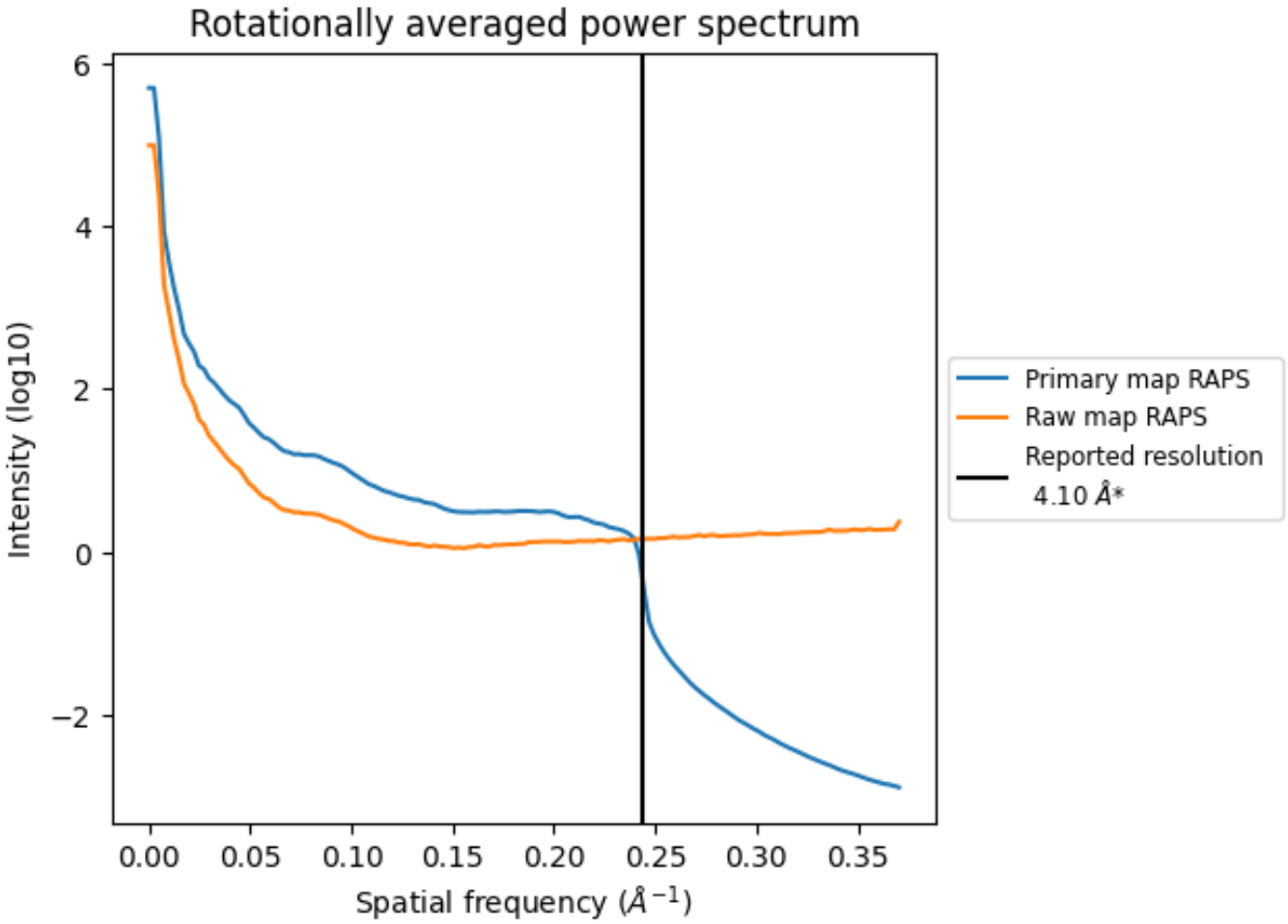
## 7.2 Volume estimate




The volume at the recommended contour level is 2180 $nm^3$; this corresponds to an approximate mass of 1970 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)

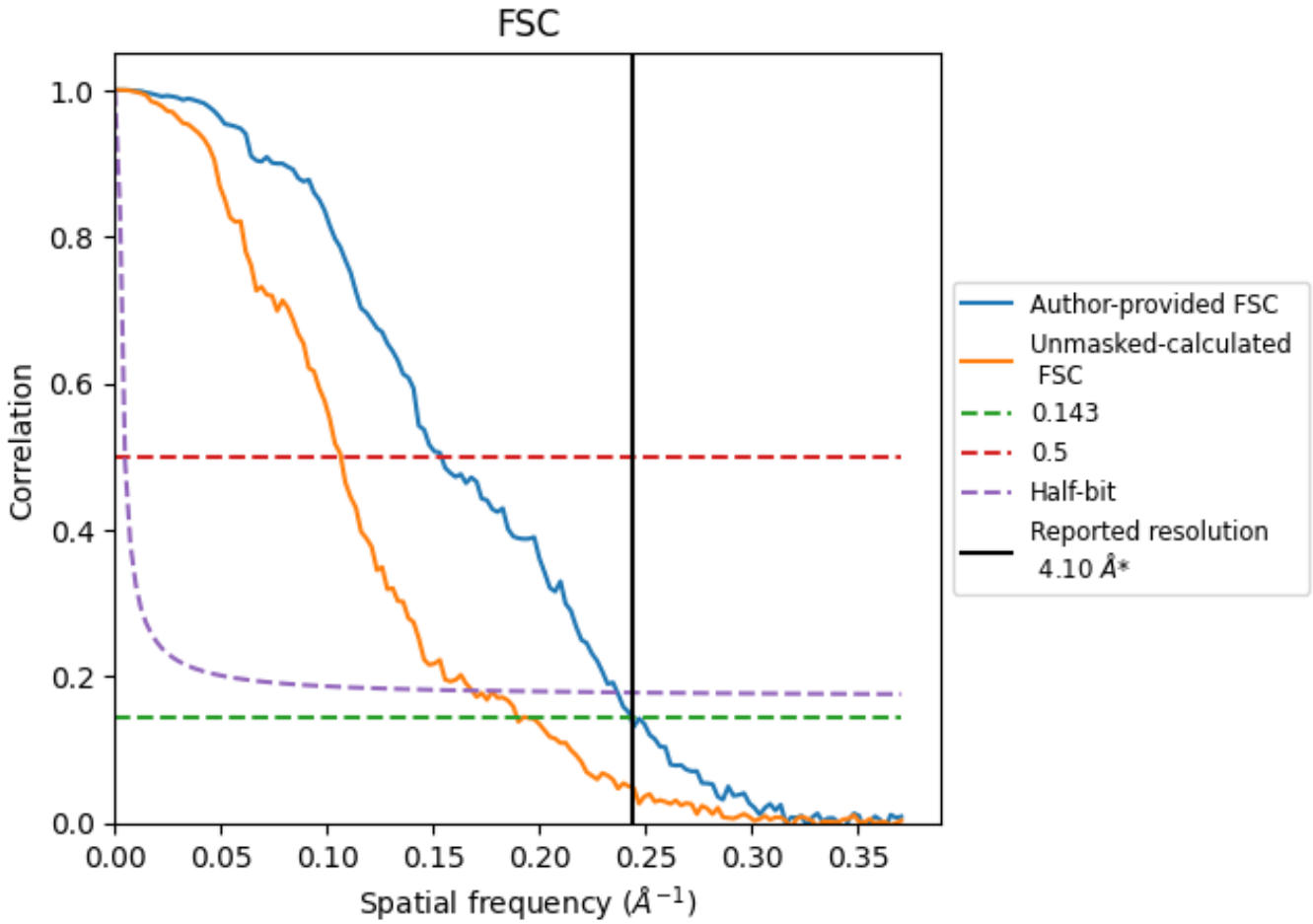



*Reported resolution corresponds to spatial frequency of 0.244 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.244 Å$^{-1}$

## 8.2 Resolution estimates (i)

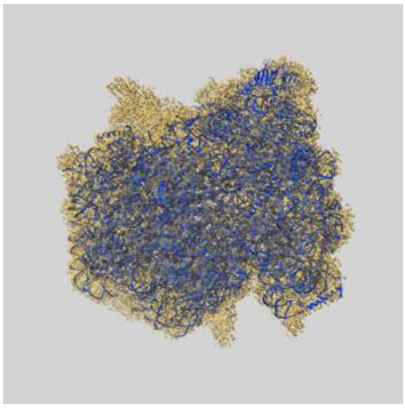
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.10 | - | - |
| Author-provided FSC curve | 4.12 | 6.51 | 4.22 |
| Unmasked-calculated* | 5.28 | 9.40 | 5.94 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.28 differs from the reported value 4.1 by more than 10 %

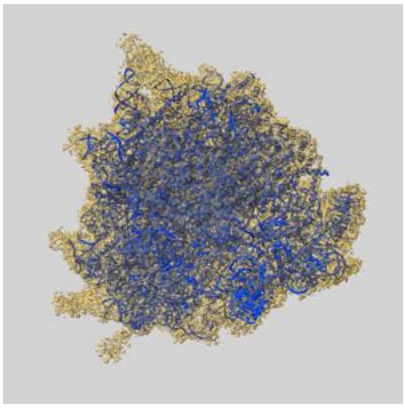
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12632 and PDB model 7NWH. Per-residue inclusion information can be found in section 3 on page 22.

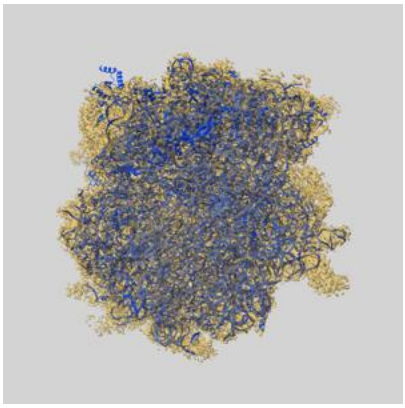
## 9.1 Map-model overlay



X



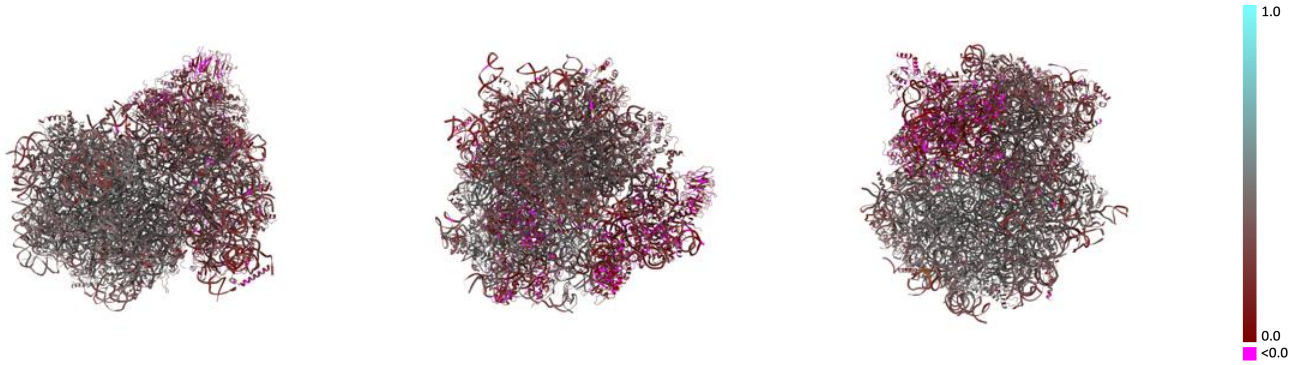
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

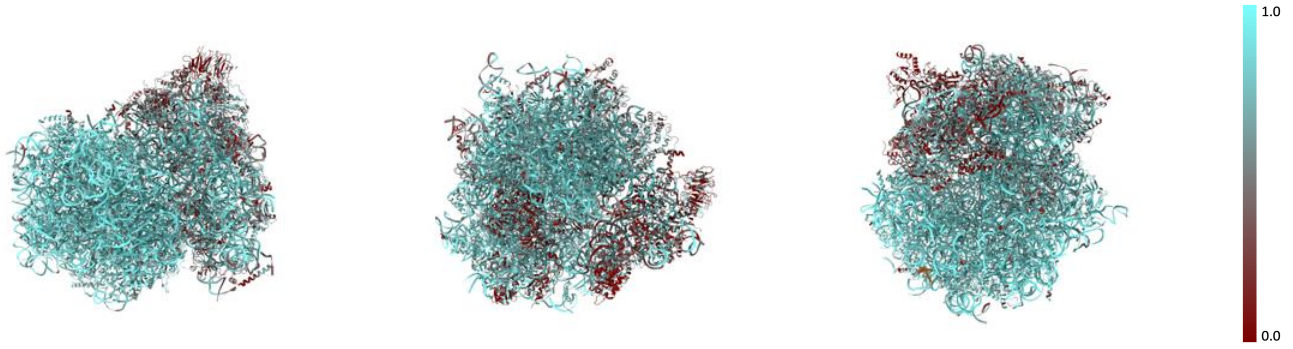
## 9.2 Q-score mapped to coordinate model (i)




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.

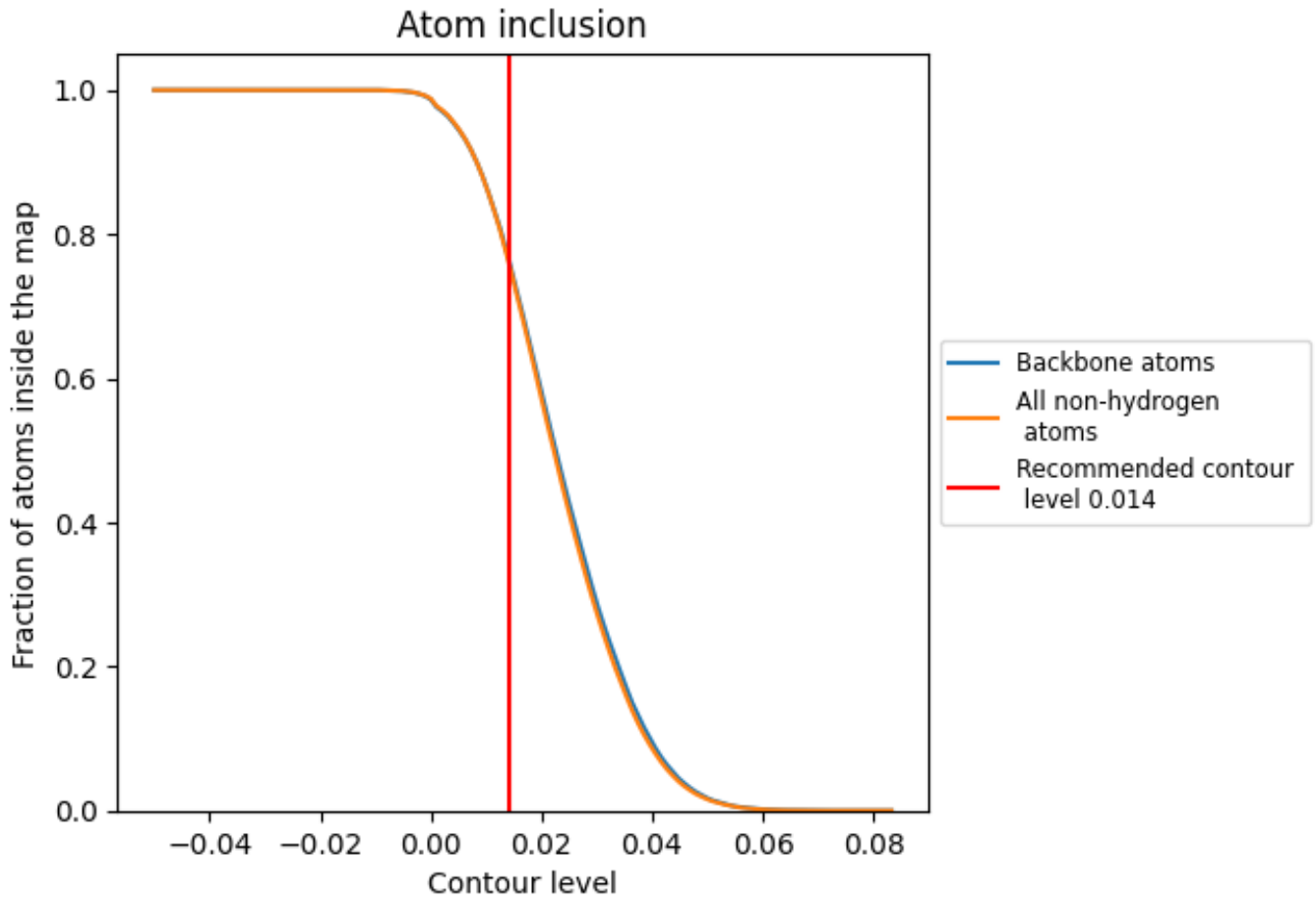
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.014).

## 9.4 Atom inclusion (i)




At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7638 | 0.3480 |
| 5 | 0.9284 | 0.3970 |
| 7 | 0.9629 | 0.4130 |
| 8 | 0.9481 | 0.4100 |
| 9 | 0.7792 | 0.2790 |
| A | 0.8125 | 0.4540 |
| AA | 0.6058 | 0.3260 |
| B | 0.8007 | 0.4370 |
| BB | 0.5574 | 0.2980 |
| C | 0.8136 | 0.4440 |
| CC | 0.6568 | 0.3580 |
| D | 0.7991 | 0.3880 |
| DD | 0.3699 | 0.2000 |
| E | 0.8023 | 0.4100 |
| EE | 0.6000 | 0.3260 |
| F | 0.8010 | 0.4240 |
| FF | 0.3401 | 0.1590 |
| G | 0.7540 | 0.3880 |
| GG | 0.5024 | 0.2420 |
| H | 0.7740 | 0.4150 |
| HH | 0.4887 | 0.2780 |
| I | 0.8055 | 0.4320 |
| II | 0.5821 | 0.3030 |
| J | 0.7540 | 0.3480 |
| JJ | 0.6526 | 0.3220 |
| KK | 0.3987 | 0.1850 |
| L | 0.7748 | 0.4060 |
| LL | 0.6596 | 0.3600 |
| M | 0.8089 | 0.4130 |
| MM | 0.0805 | 0.0870 |
| N | 0.8451 | 0.4470 |
| NN | 0.6132 | 0.3210 |
| O | 0.8186 | 0.4320 |
| OO | 0.5512 | 0.2680 |
| P | 0.8260 | 0.4440 |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| Chain | Atom inclusion | Q-score |
|---|---|---|
| PP | 0.4933 | 0.1590 |
| Q | 0.8021 | 0.4370 |
| QQ | 0.4359 | 0.1810 |
| R | 0.7495 | 0.3910 |
| RR | 0.3998 | 0.2170 |
| S | 0.8210 | 0.4420 |
| SS | 0.4812 | 0.1830 |
| T | 0.7981 | 0.4440 |
| TT | 0.4499 | 0.1640 |
| U | 0.7383 | 0.3510 |
| UU | 0.4083 | 0.1710 |
| V | 0.7724 | 0.4530 |
| VV | 0.5997 | 0.3340 |
| W | 0.5704 | 0.3100 |
| WW | 0.6485 | 0.3580 |
| X | 0.8064 | 0.4180 |
| XX | 0.7283 | 0.3910 |
| Y | 0.8089 | 0.4200 |
| YY | 0.5403 | 0.2790 |
| Z | 0.7931 | 0.3830 |
| ZZ | 0.3688 | 0.1690 |
| a | 0.8220 | 0.4490 |
| aa | 0.6624 | 0.3430 |
| b | 0.7215 | 0.3870 |
| bb | 0.5540 | 0.3160 |
| c | 0.6935 | 0.3420 |
| cc | 0.2745 | 0.1690 |
| d | 0.7783 | 0.4200 |
| dd | 0.4502 | 0.1990 |
| e | 0.8269 | 0.4580 |
| ee | 0.5915 | 0.3220 |
| f | 0.8468 | 0.4600 |
| ff | 0.3457 | 0.2120 |
| g | 0.7805 | 0.4170 |
| gg | 0.2727 | 0.1370 |
| h | 0.8018 | 0.3970 |
| hh | 0.2132 | 0.1730 |
| i | 0.7714 | 0.3880 |
| ii | 0.2776 | 0.1660 |
| j | 0.8739 | 0.4480 |
| jj | 0.2419 | 0.1590 |
| k | 0.7397 | 0.3890 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| l | 0.8361 | 0.4370 |
| m | 0.8149 | 0.4180 |
| n | 0.6284 | 0.3300 |
| o | 0.7787 | 0.4390 |
| p | 0.7939 | 0.4420 |
| r | 0.8025 | 0.4280 |
| s | 0.3246 | 0.1490 |
| t | 0.3155 | 0.1860 |