



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 06:05 AM EDT

PDB ID : 5IT7
EMDB ID: : EMD-8123
Title : Structure of the Kluyveromyces lactis 80S ribosome in complex with the cricket paralysis virus IRES and eEF2
Authors : Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.
Deposited on : unknown
Resolution : 3.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

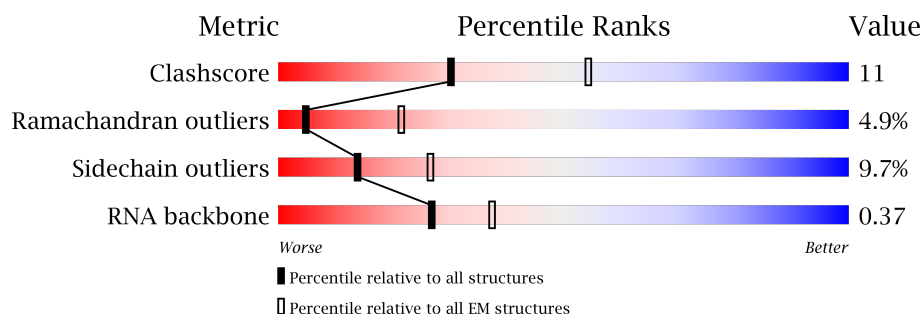
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



















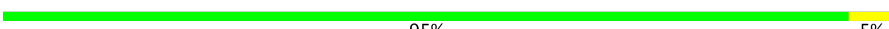





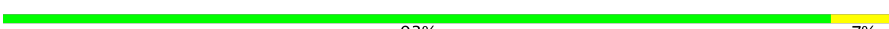


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |
| RNA backbone | 3398 | 335 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 5 | 3270 | 46% 41% 11% . |
| 2 | 7 | 121 | 63% 34% . |
| 3 | 8 | 157 | 50% 43% 5% . |
| 4 | AA | 249 | 69% 24% 6% |
| 5 | BB | 384 | 65% 28% 7% |
| 6 | CC | 360 | 68% 24% 8% |
| 7 | DD | 295 | 76% 22% . |
| 8 | EE | 170 | 76% 12% 6% . 5% |














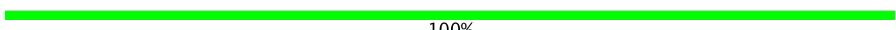











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 9 | FF | 222 |  74%19%6% |
| 10 | GG | 233 |  80%17%. |
| 11 | HH | 191 |  79%19%. |
| 12 | II | 216 |  75%19%.. |
| 13 | JJ | 168 |  81%15%. |
| 14 | LL | 197 |  79%17%. |
| 15 | MM | 136 |  79%18%. |
| 16 | NN | 202 |  77%19%. |
| 17 | OO | 198 |  10%51%35%. |
| 18 | PP | 180 |  73%22%. |
| 19 | QQ | 184 |  78%18%. |
| 20 | RR | 188 |  84%14%. |
| 21 | SS | 169 |  80%19%. |
| 22 | TT | 158 |  72%24%. |
| 23 | UU | 100 |  93%7% |
| 24 | VV | 132 |  70%23%7% |
| 25 | WW | 62 |  95%5% |
| 26 | XX | 121 |  82%16%. |
| 27 | YY | 125 |  82%15%.. |
| 28 | ZZ | 134 |  72%24%. |
| 29 | aa | 147 |  85%15% |
| 30 | bb | 57 |  95%5% |
| 31 | cc | 97 |  93%7% |
| 32 | dd | 106 |  89%11% |
| 33 | ee | 122 |  94%6% |


















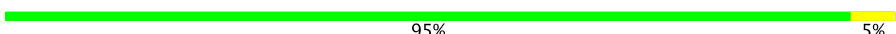
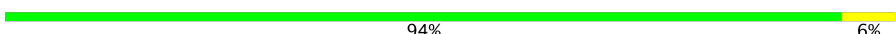






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 34 | ff | 105 |  92% 8% |
| 35 | gg | 121 |  91% 8% . |
| 36 | hh | 116 |  95% . . |
| 37 | ii | 98 |  86% 14% |
| 38 | jj | 85 |  87% 13% |
| 39 | kk | 76 |  91% 8% . |
| 40 | ll | 49 |  88% 12% |
| 41 | mm | 51 |  90% 10% |
| 42 | nn | 25 |  84% 16% |
| 43 | oo | 101 |  87% 12% . |
| 44 | pp | 87 |  77% 18% 5% |
| 45 | qq | 217 |  83% 14% . |
| 46 | rr | 195 |  85% 14% . |
| 47 | KK | 147 |  100% |
| 48 | A | 206 |  76% 19% . . |
| 49 | B | 214 |  81% 16% . |
| 50 | C | 217 |  76% 19% 5% . |
| 51 | D | 223 |  85% 12% . |
| 52 | E | 260 |  84% 13% . |
| 53 | F | 206 |  85% 14% . |
| 54 | G | 226 |  83% 15% . |
| 55 | H | 184 |  82% 17% . |
| 56 | I | 200 |  75% 19% . 6% |
| 57 | J | 182 |  74% 21% 5% |
| 58 | K | 96 |  83% 15% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 59 | L | 155 |  |
| 60 | M | 122 |  |
| 61 | N | 150 |  |
| 62 | O | 127 |  |
| 63 | P | 123 |  |
| 64 | Q | 141 |  |
| 65 | R | 129 |  |
| 66 | S | 145 |  |
| 67 | T | 143 |  |
| 68 | U | 106 |  |
| 69 | V | 87 |  |
| 70 | W | 129 |  |
| 71 | X | 145 |  |
| 72 | Y | 134 |  |
| 73 | Z | 70 |  |
| 74 | a | 100 |  |
| 75 | b | 82 |  |
| 76 | c | 63 |  |
| 77 | d | 53 |  |
| 78 | e | 55 |  |
| 79 | f | 69 |  |
| 80 | g | 324 |  |
| 81 | 2 | 1798 |  |
| 82 | 4 | 190 |  |
| 83 | 1 | 827 |  |

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is DNA/RNA hybrid called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1 | 5 | 3270 | Total | C | N | O | P | 0 | 0 |
| | | | 69896 | 31222 | 12579 | 22825 | 3270 | | |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2 | 7 | 121 | Total | C | N | O | P | 0 | 0 |
| | | | 2579 | 1152 | 461 | 845 | 121 | | |

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3 | 8 | 157 | Total | C | N | O | P | 0 | 0 |
| | | | 3326 | 1488 | 573 | 1108 | 157 | | |

- Molecule 4 is a protein called KLLA0D16027p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | AA | 249 | Total | C | N | O | S | 0 | 0 |
| | | | 1892 | 1176 | 385 | 330 | 1 | | |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | BB | 384 | Total | C | N | O | S | 0 | 0 |
| | | | 3064 | 1946 | 580 | 533 | 5 | | |

- Molecule 6 is a protein called KLLA0B07139p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | CC | 359 | Total | C | N | O | S | 0 | 0 |
| | | | 2731 | 1715 | 522 | 491 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| CC | 3 | ARG | ILE | conflict | UNP Q6CW41 |

- Molecule 7 is a protein called KLLA0D06941p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | DD | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2384 | 1510 | 417 | 456 | 1 | | |

- Molecule 8 is a protein called KLLA0B04686p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | EE | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1300 | 834 | 243 | 223 | | | |

- Molecule 9 is a protein called KLLA0D03410p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9 | FF | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1774 | 1138 | 319 | 316 | 1 | | |

- Molecule 10 is a protein called KLLA0E00573p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | GG | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1817 | 1160 | 324 | 330 | 3 | | |

- Molecule 11 is a protein called KLLA0F04499p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | HH | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1528 | 965 | 277 | 284 | 2 | | |

- Molecule 12 is a protein called KLLA0D05643p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | II | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1690 | 1074 | 319 | 292 | 5 | | |

- Molecule 13 is a protein called KLLA0F08261p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | JJ | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1349 | 845 | 255 | 245 | 4 | | |

- Molecule 14 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 14 | LL | 197 | Total | C | N | O | | 0 | 0 |
| | | | 1581 | 988 | 317 | 276 | | | |

- Molecule 15 is a protein called KLLA0B13409p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 15 | MM | 136 | Total | C | N | O | | 0 | 0 |
| | | | 1045 | 666 | 196 | 183 | | | |

- Molecule 16 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16 | NN | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1709 | 1069 | 359 | 280 | 1 | | |

- Molecule 17 is a protein called KLLA0F04675p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17 | OO | 198 | Total | C | N | O | S | 196 | 0 |
| | | | 1571 | 1013 | 290 | 267 | 1 | | |

- Molecule 18 is a protein called KLLA0A06336p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 18 | PP | 180 | Total | C | N | O | | 0 | 0 |
| | | | 1432 | 885 | 287 | 260 | | | |

- Molecule 19 is a protein called KLLA0A07227p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 19 | QQ | 184 | Total | C | N | O | | 0 | 0 |
| | | | 1444 | 911 | 290 | 243 | | | |

- Molecule 20 is a protein called KLLA0E12453p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | RR | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1522 | 933 | 328 | 259 | 2 | | |

- Molecule 21 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | SS | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1416 | 916 | 259 | 238 | 3 | | |

- Molecule 22 is a protein called KLLA0E23651p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | TT | 158 | Total | C | N | O | S | 0 | 0 |
| | | | 1262 | 797 | 240 | 220 | 5 | | |

- Molecule 23 is a protein called KLLA0D05181p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 23 | UU | 100 | Total | C | N | O | 0 | 0 |
| | | | 807 | 524 | 131 | 152 | | |

- Molecule 24 is a protein called KLLA0E06997p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | VV | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 612 | 182 | 174 | 8 | | |

- Molecule 25 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 25 | WW | 62 | Total | C | N | O | 0 | 0 |
| | | | 515 | 330 | 103 | 82 | | |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | XX | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 620 | 169 | 174 | 1 | | |

- Molecule 27 is a protein called KLLA0B05742p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 27 | YY | 125 | Total | C | N | O | 0 | 0 |
| | | | 992 | 622 | 189 | 181 | | |

- Molecule 28 is a protein called KLLA0E03455p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 28 | ZZ | 134 | Total | C | N | O | 0 | 0 |
| | | | 1089 | 708 | 199 | 182 | | |

- Molecule 29 is a protein called RPL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | aa | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1156 | 740 | 225 | 189 | 2 | | |

- Molecule 30 is a protein called KLLA0D16071p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 30 | bb | 57 | Total | C | N | O | 0 | 0 |
| | | | 458 | 287 | 99 | 72 | | |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | cc | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 477 | 125 | 137 | 1 | | |

- Molecule 32 is a protein called KLLA0B02937p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | dd | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 869 | 553 | 167 | 147 | 2 | | |

- Molecule 33 is a protein called KLLA0E06843p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | ee | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 980 | 618 | 198 | 162 | 2 | | |

- Molecule 34 is a protein called KLLA0D07405p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | ff | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 837 | 531 | 161 | 144 | 1 | | |

- Molecule 35 is a protein called KLLA0C08371p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | gg | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 951 | 591 | 192 | 167 | 1 | | |

- Molecule 36 is a protein called KLLA0F05247p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 36 | hh | 116 | Total | C | N | O | 0 | 0 |
| | | | 961 | 608 | 187 | 166 | | |

- Molecule 37 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | ii | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 479 | 155 | 131 | 1 | | |

- Molecule 38 is a protein called Ribosomal protein L37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | jj | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 675 | 410 | 148 | 111 | 6 | | |

- Molecule 39 is a protein called KLLA0C18216p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39 | kk | 76 | Total | C | N | O | 0 | 0 |
| | | | 619 | 398 | 114 | 107 | | |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40 | ll | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 428 | 266 | 96 | 64 | 2 | | |

- Molecule 41 is a protein called Ubiquitin fusion protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41 | mm | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 410 | 254 | 85 | 66 | 5 | | |

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42 | nn | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | |

- Molecule 43 is a protein called 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | oo | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 814 | 509 | 163 | 136 | 6 | | |

- Molecule 44 is a protein called KLLA0E05941p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | pp | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 660 | 404 | 133 | 117 | 6 | | |

- Molecule 45 is a protein called Ribosomal protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | qq | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1100 | 300 | 312 | 9 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| qq | 11 | GLU | ASP | conflict | UNP Q6CWR9 |
| qq | 12 | HIS | ASN | conflict | UNP Q6CWR9 |
| qq | 152 | ARG | LYS | conflict | UNP Q6CWR9 |

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | rr | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1508 | 968 | 258 | 278 | 4 | | |

- Molecule 47 is a protein called uL11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 47 | KK | 147 | Total | C | N | O | 0 | 0 |
| | | | 735 | 441 | 147 | 147 | | |

- Molecule 48 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48 | A | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1616 | 1035 | 285 | 294 | 2 | | |

- Molecule 49 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49 | B | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1722 | 1089 | 313 | 317 | 3 | | |

- Molecule 50 is a protein called KLLA0F09812p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50 | C | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1629 | 1041 | 287 | 297 | 4 | | |

- Molecule 51 is a protein called KLLA0D08305p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51 | D | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1744 | 1108 | 313 | 318 | 5 | | |

- Molecule 52 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52 | E | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2078 | 1322 | 393 | 359 | 4 | | |

- Molecule 53 is a protein called KLLA0D10659p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53 | F | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1609 | 1008 | 298 | 300 | 3 | | |

- Molecule 54 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54 | G | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1134 | 348 | 326 | 4 | | |

- Molecule 55 is a protein called KLLA0C13519p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 55 | H | 184 | Total | C | N | O | | 0 | 0 |
| | | | 1483 | 950 | 270 | 263 | | | |

- Molecule 56 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56 | I | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1493 | 926 | 301 | 265 | 1 | | |

- Molecule 57 is a protein called KLLA0E23673p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57 | J | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1471 | 929 | 287 | 254 | 1 | | |

- Molecule 58 is a protein called KLLA0B08173p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58 | K | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 809 | 533 | 129 | 146 | 1 | | |

- Molecule 59 is a protein called KLLA0A10483p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59 | L | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1248 | 798 | 237 | 210 | 3 | | |

- Molecule 60 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 60 | M | 122 | Total | C | N | O | | 0 | 0 |
| | | | 922 | 575 | 167 | 180 | | | |

- Molecule 61 is a protein called KLLA0F18040p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | N | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 756 | 223 | 206 | 2 | | |

- Molecule 62 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62 | O | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 578 | 188 | 173 | 3 | | |

- Molecule 63 is a protein called KLLA0F07843p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63 | P | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 980 | 628 | 179 | 168 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| P | 130 | ALA | - | expression tag | UNP Q6CKV4 |

- Molecule 64 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 64 | Q | 141 | Total | C | N | O | 0 | 0 |
| | | | 1105 | 709 | 204 | 192 | | |

- Molecule 65 is a protein called KLLA0B01474p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65 | R | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1031 | 641 | 193 | 194 | 3 | | |

- Molecule 66 is a protein called KLLA0B01562p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66 | S | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 741 | 240 | 210 | 2 | | |

- Molecule 67 is a protein called KLLA0A07194p.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 67 | T | 143 | Total | C | N | O | 0 | 0 |
| | | | 1110 | 693 | 210 | 207 | | |

- Molecule 68 is a protein called KLLA0F25542p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68 | U | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 845 | 540 | 152 | 152 | 1 | | |

- Molecule 69 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69 | V | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 687 | 424 | 126 | 135 | 2 | | |

- Molecule 70 is a protein called 40S ribosomal protein S22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70 | W | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 651 | 187 | 180 | 3 | | |

- Molecule 71 is a protein called RPS23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71 | X | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 713 | 219 | 192 | 3 | | |

- Molecule 72 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 72 | Y | 134 | Total | C | N | O | 0 | 0 |
| | | | 1061 | 665 | 207 | 189 | | |

- Molecule 73 is a protein called KLLA0B06182p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 73 | Z | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 558 | 355 | 104 | 98 | 1 | | |

- Molecule 74 is a protein called KLLA0D05115p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74 | a | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 798 | 491 | 170 | 131 | 6 | | |

- Molecule 75 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75 | b | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 617 | 384 | 113 | 114 | 6 | | |

- Molecule 76 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 76 | c | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 494 | 305 | 98 | 90 | 1 | | |

- Molecule 77 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 77 | d | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 446 | 280 | 89 | 76 | 1 | | |

- Molecule 78 is a protein called KLLA0C04809p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78 | e | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 443 | 276 | 90 | 76 | 1 | | |

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 79 | f | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 352 | 102 | 91 | 4 | | |

- Molecule 80 is a protein called KLLA0E12277p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 80 | g | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2466 | 1561 | 430 | 470 | 5 | | |

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 81 | 2 | 1780 | Total | C | N | O | P | 0 | 0 |
| | | | 37797 | 16892 | 6658 | 12467 | 1780 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| 2 | 676 | G | U | conflict | GB 49642208 |
| 2 | 678 | U | G | conflict | GB 49642208 |

- Molecule 82 is DNA/RNA hybrid called cricket paralysis virus IRES.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 82 | 4 | 190 | Total | C | N | O | P | 0 | 0 |
| | | | 3950 | 1768 | 667 | 1325 | 190 | | |

- Molecule 83 is a protein called Eft2p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 83 | 1 | 827 | Total | C | N | O | S | 0 | 0 |
| | | | 6421 | 4070 | 1106 | 1216 | 29 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 1 | 310 | GLU | ASP | conflict | UNP W7R097 |

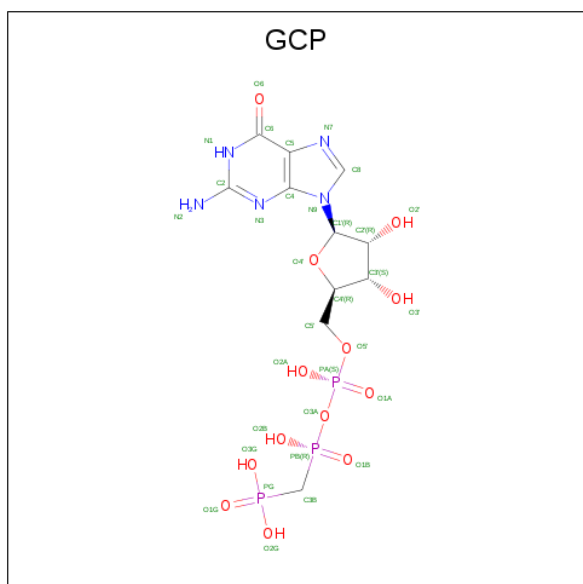
- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 84 | 2 | 75 | Total | Mg | 0 |
| | | | 75 | 75 | |
| 84 | 1 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 84 | f | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 84 | N | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 84 | 5 | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |

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

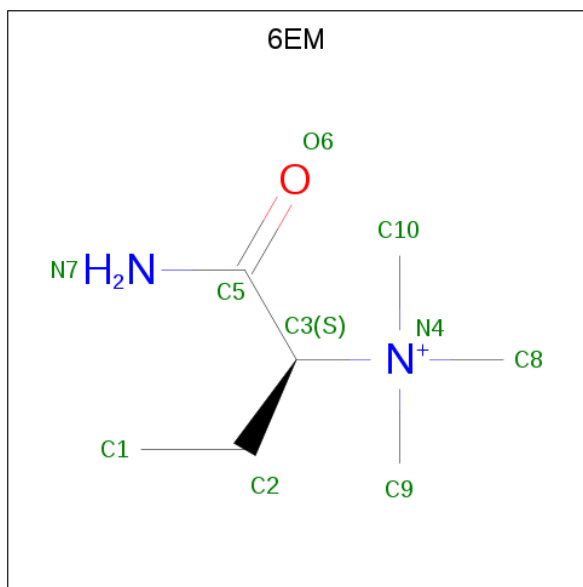
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 85 | oo | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | b | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | mm | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | jj | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | a | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 85 | f | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 86 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 11 | 5 | 13 | 3 | |

- Molecule 87 is (2S)-1-amino-N,N,N-trimethyl-1-oxobutan-2-aminium (three-letter code: 6EM) (formula: $C_7H_{17}N_2O$).

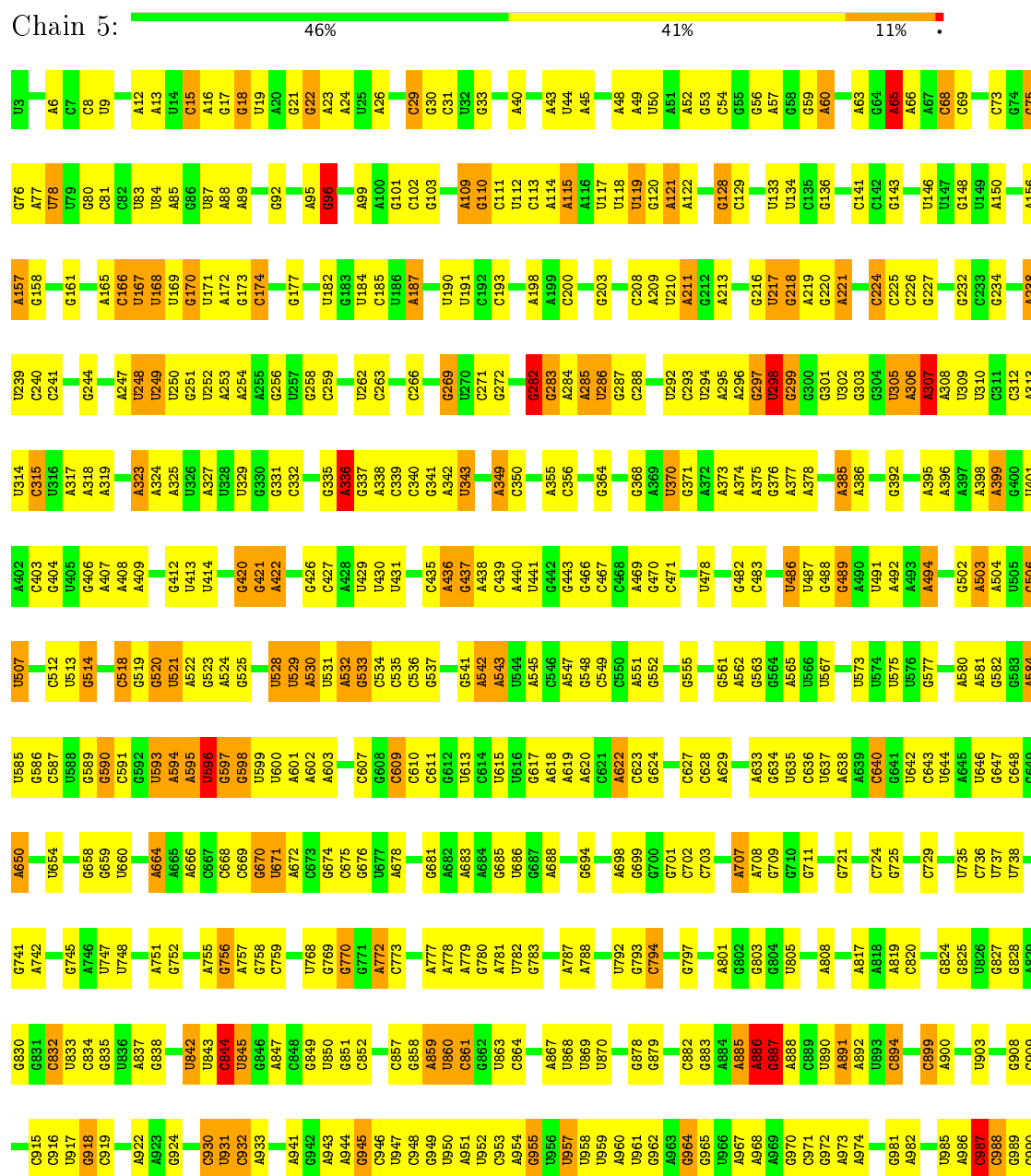


| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| | | | Total | C | N | O | |
| 87 | 1 | 1 | 10 | 7 | 2 | 1 | 0 |

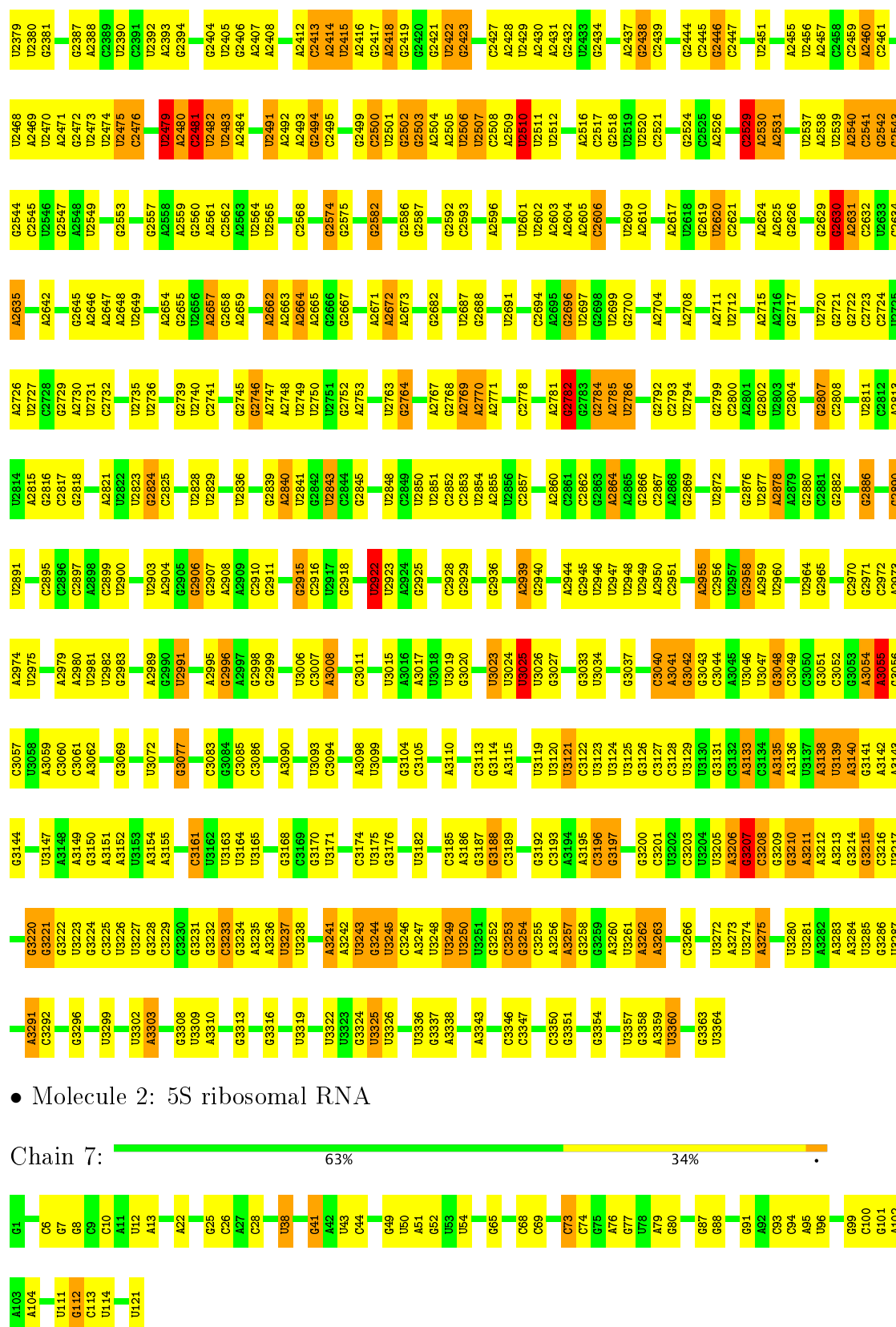
3 Residue-property plots

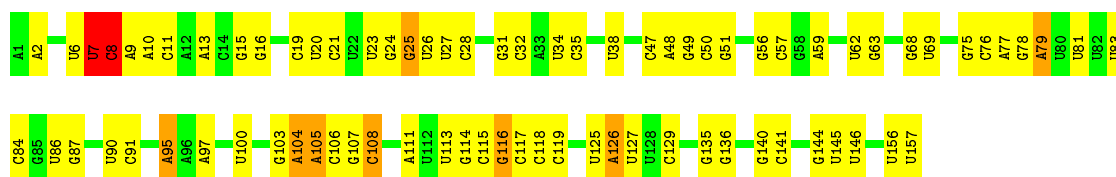
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: 25S ribosomal RNA



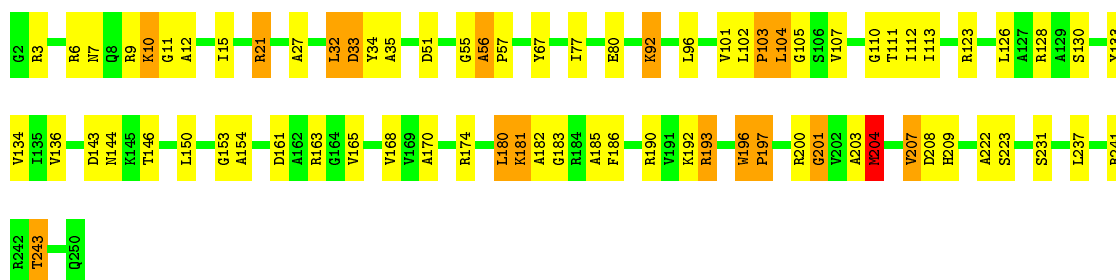
| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--|-------|
| C2309 | G2222 | A2137 | G2049 | C1791 | A1718 | G1630 | G1585 | G1481 | G1315 | G1233 | C1158 | | G991 |
| C2300 | U2223 | G2138 | G2049 | A1792 | A1719 | G1631 | A1558 | G1484 | G1316 | A1234 | U1159 | | G992 |
| A2301 | A2224 | U2139 | A2050 | G1793 | A1720 | C1632 | A1558 | G1485 | G1317 | U1235 | C1160 | | G993 |
| C2302 | A2225 | G2140 | U2051 | G1794 | A1721 | G1633 | G1559 | G1486 | U1318 | U1236 | A1161 | | U994 |
| U2303 | C2226 | C1873 | G2052 | C1795 | C1723 | C1634 | G1560 | G1487 | U1319 | G1237 | U1162 | | G995 |
| G2304 | U2227 | G1874 | C2053 | C1796 | C1724 | G1637 | G1561 | G1491 | A1320 | | C1163 | | G996 |
| U2305 | A2228 | C1150 | U2054 | A1797 | G1725 | C1638 | A1562 | G1492 | A1321 | G1248 | C1164 | | A997 |
| | U2229 | A2151 | G2055 | G1798 | C1726 | | A1563 | G1493 | U1409 | | U1166 | | A998 |
| C2308 | G2230 | G2155 | C2056 | G1799 | A1727 | U1641 | U1564 | U1494 | A1322 | C1250 | G1167 | | U999 |
| U2313 | A2231 | U2155 | A2057 | U1800 | G1728 | G1642 | C1565 | G1496 | U1324 | | U1092 | | G1000 |
| A2314 | C2232 | G2156 | A2058 | C1801 | C1729 | U1643 | A1572 | U1497 | A1325 | C1254 | A1168 | | G1003 |
| U2316 | U2233 | U2159 | U2059 | G1807 | G1730 | G1643 | U1573 | A1498 | A1326 | G1255 | C1172 | | U1004 |
| | C2234 | U2160 | U2060 | A1808 | U1731 | G1644 | A1574 | G1499 | G1328 | A1257 | A1173 | | U1005 |
| G2324 | U2235 | C2161 | C2061 | A1809 | U1732 | U1645 | U1575 | | C1329 | A1258 | A1174 | | G1006 |
| A2325 | U2237 | U2162 | A2062 | A1810 | G1733 | G1646 | U1576 | C1503 | G1333 | A1261 | G1177 | | A1017 |
| C2326 | G2238 | G2163 | C2063 | A1811 | U1734 | U1651 | C1577 | U1504 | A1334 | A1262 | A1106 | | A1018 |
| A2326 | A2239 | C2164 | G2064 | C1812 | G1735 | A1652 | C1578 | G1507 | A1335 | C1263 | U1179 | | A1019 |
| A2327 | C2240 | G2165 | A2065 | | | | G1579 | | G1336 | G1180 | C1108 | | C1020 |
| C2328 | G2241 | C2166 | A2069 | C1815 | G1739 | U1656 | G1580 | A1510 | A1337 | G1266 | U1109 | | A1025 |
| | G2242 | A2167 | C2070 | A1816 | | U1657 | A1581 | A1510 | A1425 | C1267 | U1186 | | A1026 |
| C2331 | U2243 | G2168 | U2071 | G1817 | C1742 | U1658 | C1584 | G1513 | G1338 | G1268 | G1110 | | |
| A2332 | A2244 | U2169 | U2072 | C1818 | G1743 | | U1585 | G1514 | U1339 | C1269 | G1111 | | |
| G2333 | G2245 | G2170 | A2073 | A1819 | G1744 | U1664 | G1586 | G1515 | A1340 | | C1112 | | |
| | C2246 | C2171 | | | | A1665 | G1587 | | G1346 | A1272 | G1113 | | G1030 |
| A2336 | C2247 | U2172 | C2077 | C1823 | G1747 | A1666 | G1588 | | C1347 | A1273 | A1114 | | U1031 |
| | A2248 | C2173 | U2078 | U1824 | C1748 | | A1589 | C1521 | G1350 | U1274 | U1115 | | A1032 |
| C2339 | U2249 | U2174 | G2079 | C1825 | G1749 | C1670 | A1590 | C1522 | A1351 | A1275 | G1116 | | A1033 |
| C2340 | A2250 | G2175 | C2080 | A1826 | C1750 | U1671 | | U1524 | G1352 | A1194 | G1119 | | G1034 |
| A2341 | U2251 | C1924 | U2081 | A1827 | C1751 | U1672 | C1597 | U1525 | A1352 | C1277 | G1120 | | A1035 |
| C2342 | G2252 | A1828 | A2082 | A1828 | C1752 | U1673 | U1598 | U1526 | G1353 | G1278 | A1121 | | A1036 |
| | | U1926 | C2083 | | C1753 | U1674 | U1599 | C1527 | G1354 | | G1197 | | |
| C2343 | C2253 | C1811 | | A1833 | G1754 | | A1446 | | U1355 | A1280 | C1198 | | G1043 |
| G2344 | U2254 | A1834 | A2086 | A1834 | G1755 | C1678 | C1600 | A1528 | C1356 | G1281 | A1122 | | U1044 |
| G2345 | A2255 | C1835 | C2087 | A1835 | A1756 | C1679 | A1601 | A1529 | A1357 | A1282 | A1124 | | U1045 |
| C2346 | U2256 | A1836 | G2088 | A1836 | G1757 | | G1602 | A1530 | | C1283 | A1125 | | |
| C2347 | C2257 | G1837 | G2089 | G1837 | U1763 | A1684 | G1603 | A1531 | A1361 | G1284 | C1126 | | U1049 |
| | A2258 | U1764 | A2090 | | U1765 | U1685 | G1604 | G1532 | | | C1127 | | |
| C2352 | U2259 | C1942 | G2091 | U1840 | A1766 | G1687 | C1608 | C1533 | A1370 | A1288 | G1128 | | U1052 |
| G2354 | G2092 | C1943 | G2092 | U1841 | C1767 | U1686 | G1609 | C1534 | G1371 | A1289 | A1129 | | U1053 |
| | C2093 | G2025 | G2093 | A1844 | A1769 | U1688 | U1610 | U1535 | G1457 | C1209 | A1130 | | G1054 |
| U2357 | A2094 | C2027 | A2094 | U1845 | U1770 | U1689 | A1611 | A1537 | G1458 | G1290 | C1210 | | A1055 |
| C2358 | A2095 | G2028 | G2095 | U1846 | U1771 | U1690 | A1612 | U1538 | G1459 | C1291 | U1138 | | G1056 |
| | A2100 | U2029 | G2096 | G1847 | A1773 | A1692 | C1613 | U1539 | A1378 | U1296 | U1212 | | C1057 |
| | U2106 | C2030 | | A1848 | C1774 | U1693 | U1614 | U1540 | | A1297 | G1213 | | G1058 |
| | A2107 | U2032 | | U1849 | G1777 | C1694 | A1615 | C1542 | U1386 | C1298 | A1141 | | A1064 |
| A2108 | A2108 | U2033 | G2034 | A1850 | G1777 | C1694 | A1616 | U1543 | U1387 | A1216 | G1146 | | U1065 |
| | A2111 | G2035 | G2034 | A1855 | G1780 | A1701 | A1617 | A1544 | A1390 | U1300 | C1147 | | U1066 |
| | A2112 | U2036 | G2035 | U1859 | G1781 | G1704 | U1618 | G1545 | | A1301 | G1148 | | U1067 |
| A2113 | A2113 | C2037 | U2036 | A1860 | A1782 | G1705 | G1621 | G1546 | G1393 | G1221 | G1149 | | G1068 |
| A2114 | A2114 | G2038 | A2037 | G1861 | A1783 | G1706 | G1622 | C1547 | C1394 | A1222 | G1150 | | A1069 |
| G2216 | G2038 | G2039 | G1862 | U1784 | U1784 | | A1623 | C1548 | C1395 | A1223 | A1151 | | G1072 |
| | U2040 | U1863 | A1862 | A1785 | A1785 | A1710 | G1624 | A1549 | U1396 | U1224 | U1152 | | A1073 |
| C2217 | G2126 | U2040 | U1863 | G1786 | G1786 | G1713 | A1625 | A1549 | C1397 | C1225 | A1153 | | A1074 |
| G2218 | A2127 | C2041 | A1864 | U1787 | U1787 | C1714 | C1626 | C1551 | U1398 | C1307 | C1154 | | G1075 |
| G2219 | U2042 | U2042 | A1865 | U1788 | U1788 | | G1627 | C1552 | A1399 | U1312 | A1155 | | A1076 |
| A2221 | | G2046 | G1866 | U1789 | U1789 | G1717 | U1628 | U1553 | C1479 | C1313 | C1156 | | G1077 |
| | | | G1867 | U1790 | U1790 | | C1629 | C1554 | U1401 | A1314 | G1157 | | C1078 |





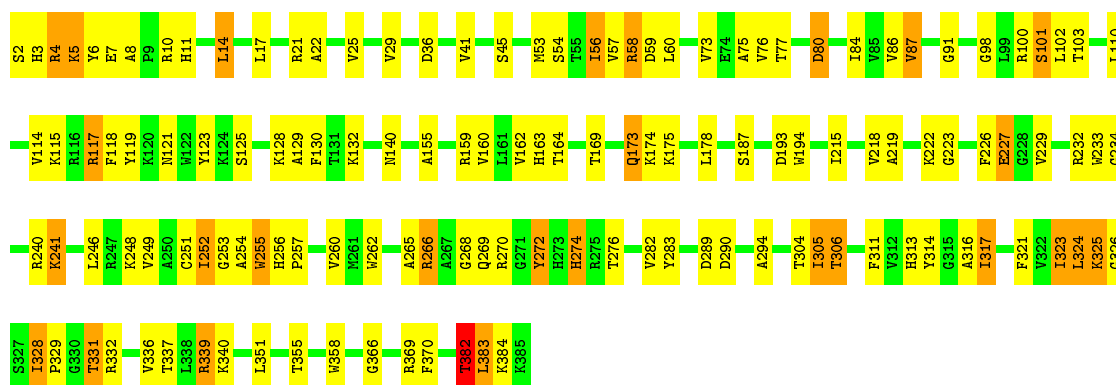
• Molecule 4: KLLA0D16027p

Chain AA: 69% 24% 6%



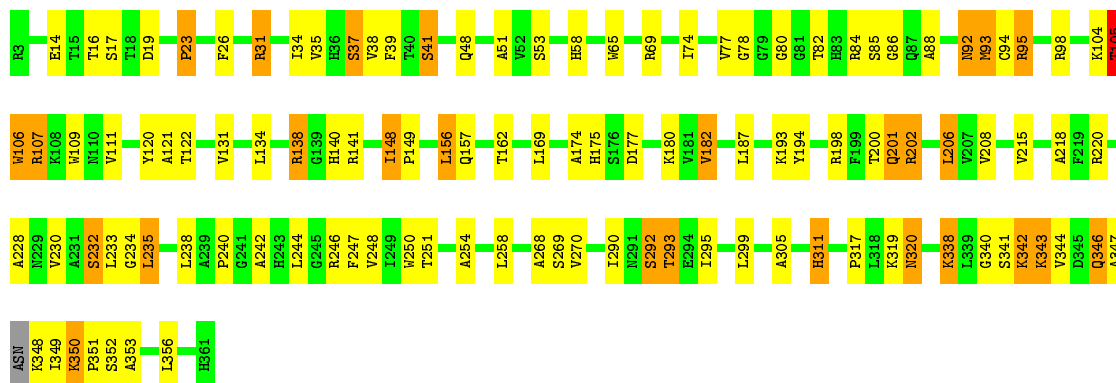
• Molecule 5: 60S ribosomal protein L3

Chain BB: 65% 28% 7%

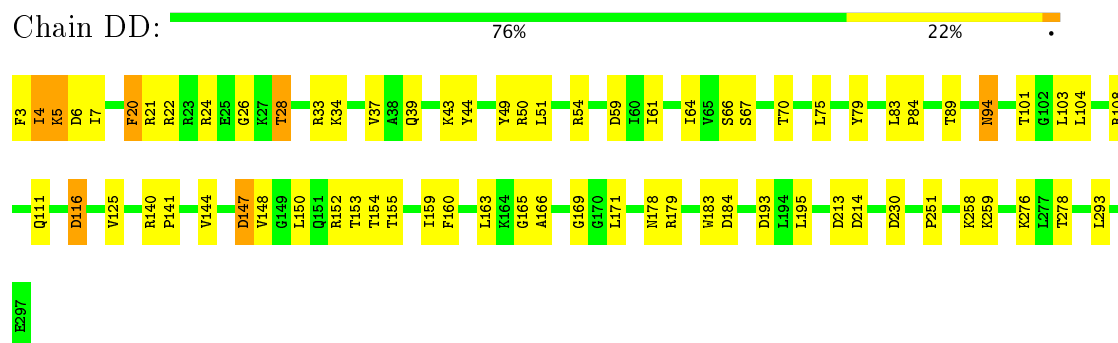


• Molecule 6: KLLA0B07139p

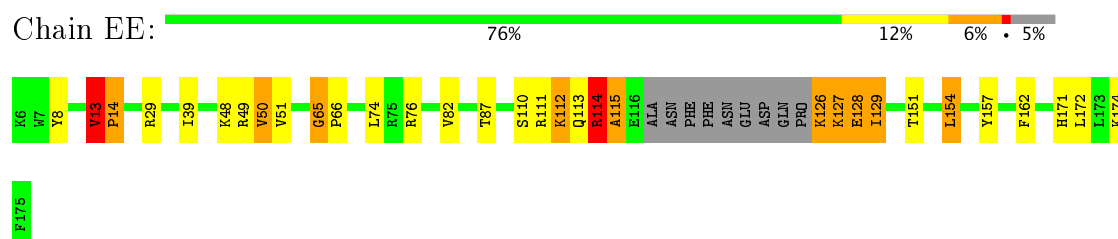
Chain CC: 68% 24% 8%



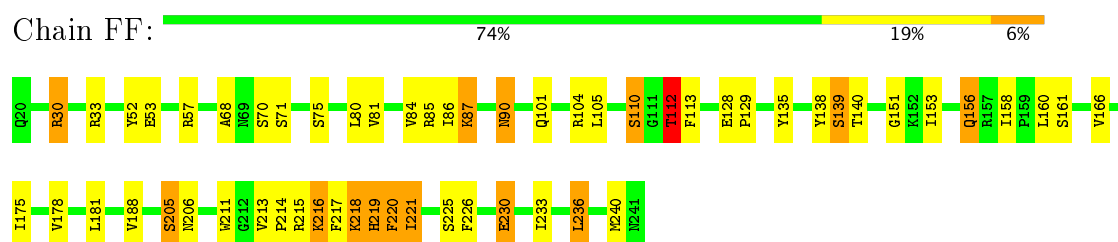
• Molecule 7: KLLA0D06941p



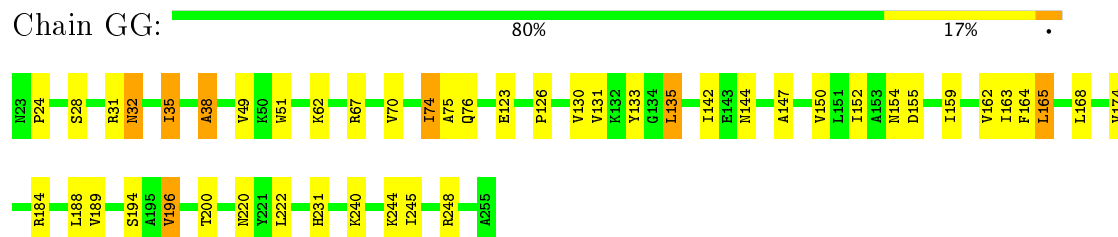
- Molecule 8: KLLA0B04686p



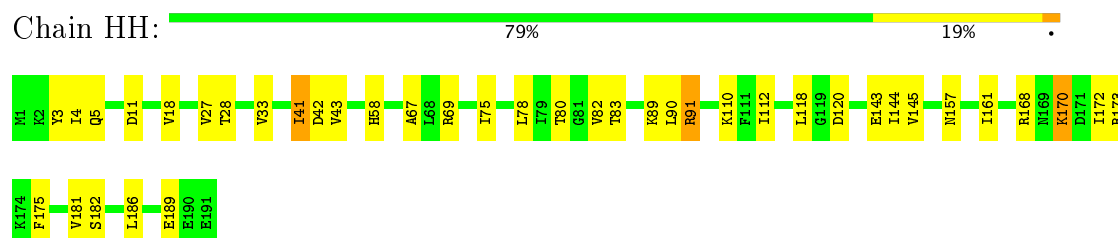
- Molecule 9: KLLA0D03410p



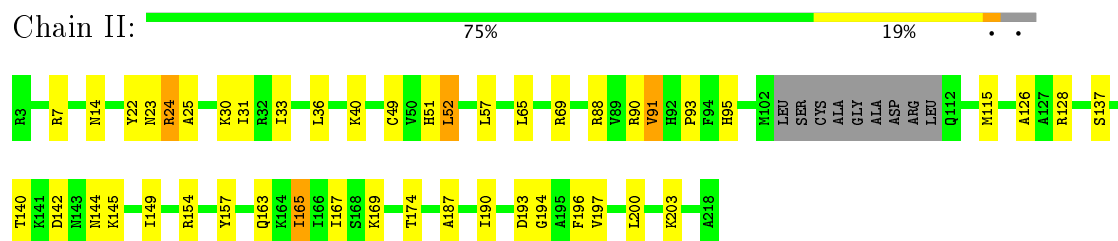
- Molecule 10: KLLA0E00573p



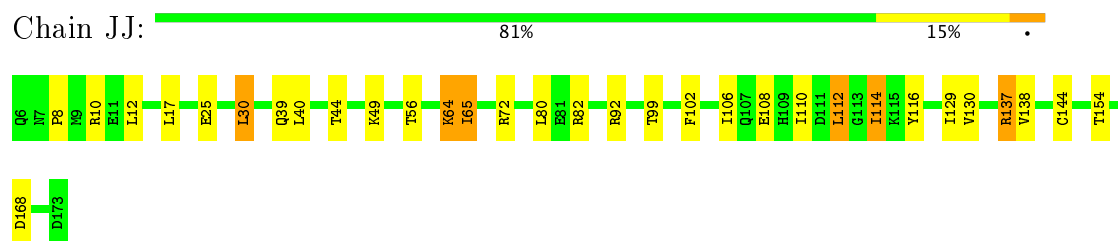
- Molecule 11: KLLA0F04499p



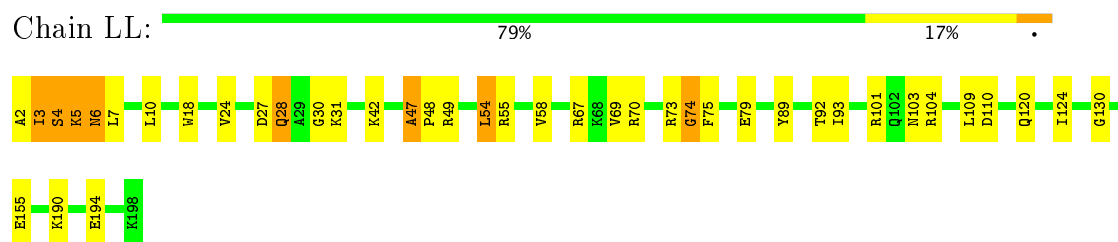
- Molecule 12: KLLA0D05643p



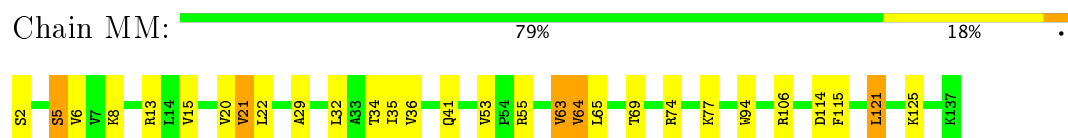
- Molecule 13: KLLA0F08261p



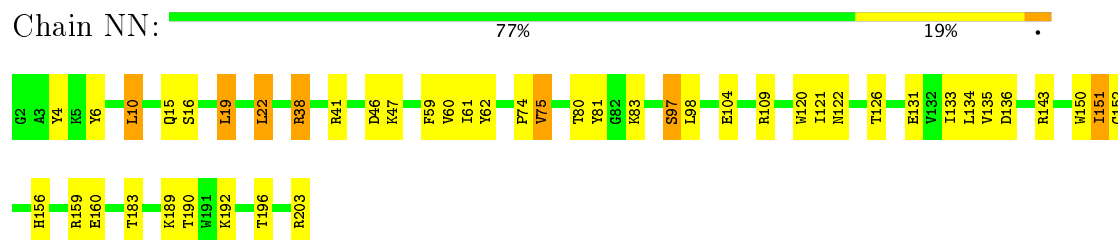
- Molecule 14: 60S ribosomal protein L13



- Molecule 15: KLLA0B13409p

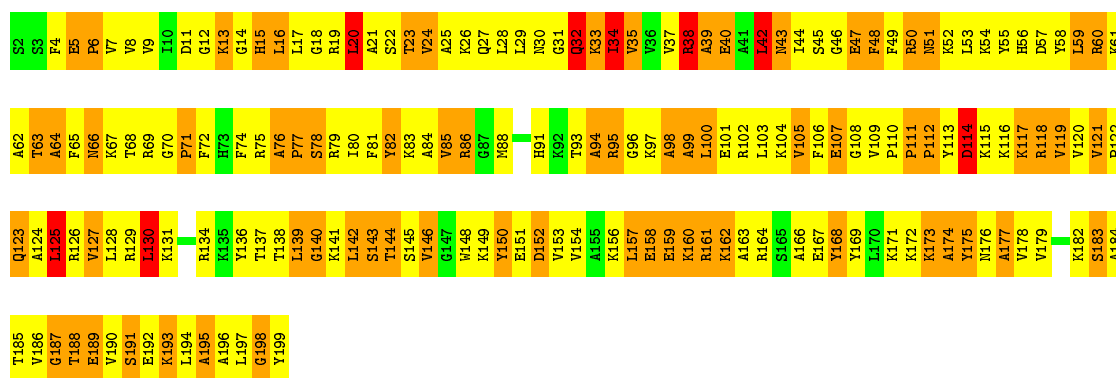


- Molecule 16: Ribosomal protein L15



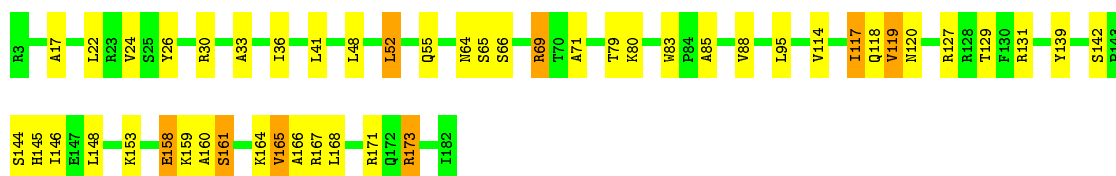
- Molecule 17: KLLA0F04675p





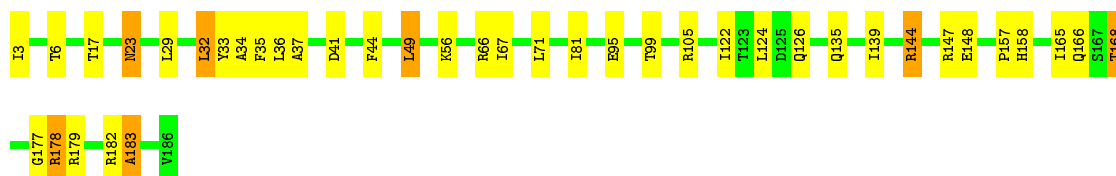
• Molecule 18: KLLA0A06336p

Chain PP: 73% 22% .



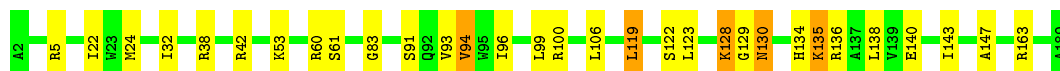
• Molecule 19: KLLA0A07227p

Chain QQ: 78% 18% .



• Molecule 20: KLLA0E12453p

Chain RR: 84% 14% .



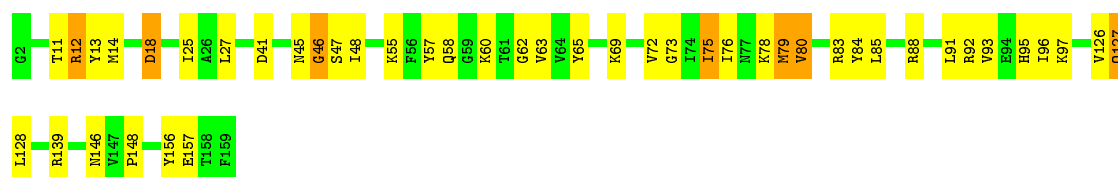
• Molecule 21: 60S ribosomal protein L20

Chain SS: 80% 19% .



• Molecule 22: KLLA0E23651p

Chain TT: 72% 24% .



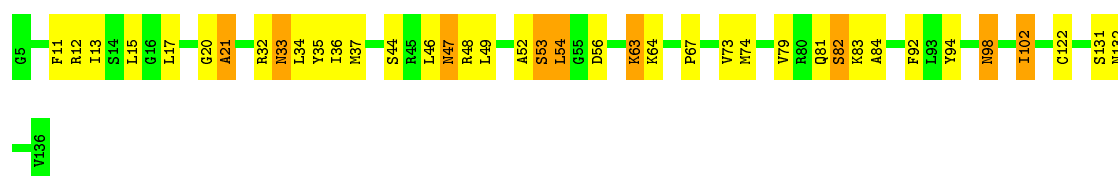
- Molecule 23: KLLA0D05181p

Chain UU: 93% 7%



- Molecule 24: KLLA0E06997p

Chain VV: 70% 23% 7%



- Molecule 25: 60S ribosomal protein L24

Chain WW: 95% 5%



- Molecule 26: 60S ribosomal protein L25

Chain XX: 82% 16% 2%



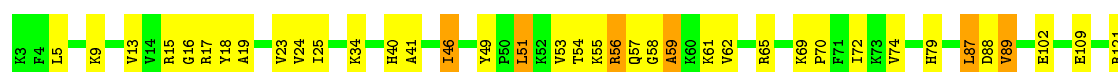
- Molecule 27: KLLA0B05742p

Chain YY: 82% 15% 3%



- Molecule 28: KLLA0E03455p

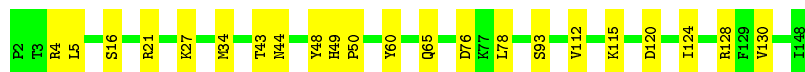
Chain ZZ: 72% 24% 4%





- Molecule 29: RPL28

Chain aa:  85% 15%



- Molecule 30: KLLA0D16071p

Chain bb:  95% 5%



- Molecule 31: 60S ribosomal protein L30

Chain cc:  93% 7%



- Molecule 32: KLLA0B02937p

Chain dd:  89% 11%



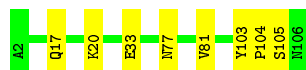
- Molecule 33: KLLA0E06843p

Chain ee:  94% 6%



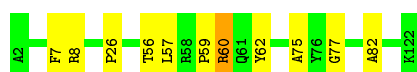
- Molecule 34: KLLA0D07405p

Chain ff:  92% 8%

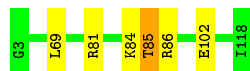


- Molecule 35: KLLA0C08371p

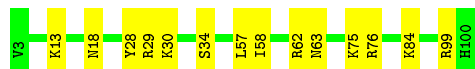
Chain gg:  91% 8%




• Molecule 36: KLLA0F05247p

Chain hh:  95% ..

• Molecule 37: 60S ribosomal protein L36

Chain ii:  86% 14%


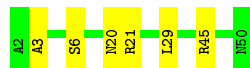
• Molecule 38: Ribosomal protein L37

Chain jj:  87% 13%

• Molecule 39: KLLA0C18216p

Chain kk:  91% 8% .


• Molecule 40: 60S ribosomal protein L39

Chain ll:  88% 12%


• Molecule 41: Ubiquitin fusion protein

Chain mm:  90% 10%

• Molecule 42: 60S ribosomal protein L41-A


Chain nn:  84% 16%

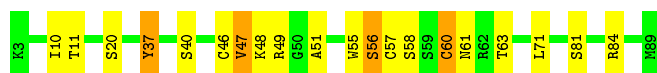
• Molecule 43: 60S ribosomal protein L44

Chain oo:  87% 12% .




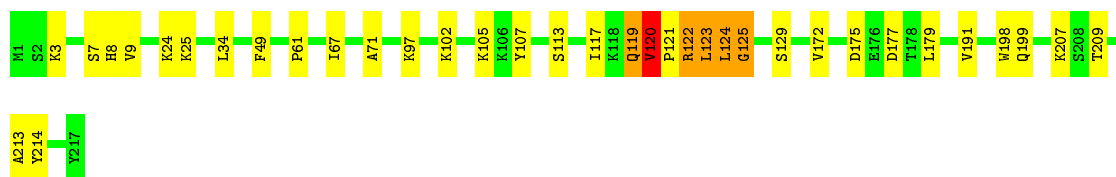
- Molecule 44: KLLA0E05941p

Chain pp:  77% 18% 5%




- Molecule 45: Ribosomal protein

Chain qq:  83% 14% .



- Molecule 46: 60S acidic ribosomal protein P0

Chain rr:  85% 14% .



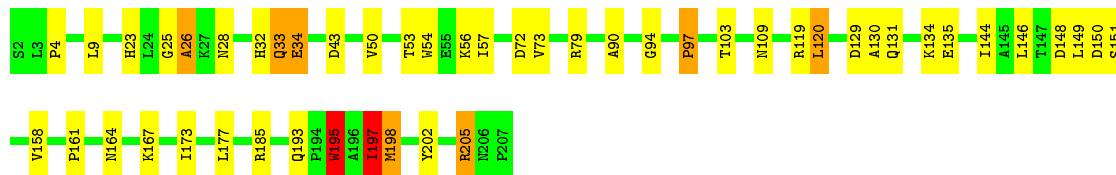
- Molecule 47: uL11

Chain KK:  100%


There are no outlier residues recorded for this chain.

- Molecule 48: 40S ribosomal protein S0

Chain A:  76% 19% . .



- Molecule 49: 40S ribosomal protein S1

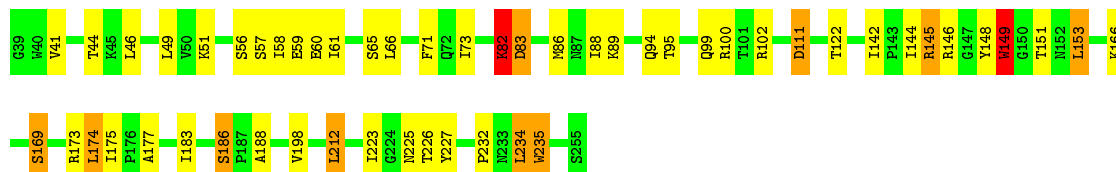
Chain B:  81% 16% .





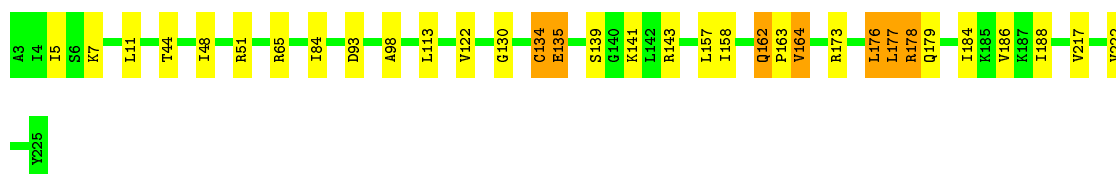
• Molecule 50: KLLA0F09812p

Chain C: 76% 19% 5% •



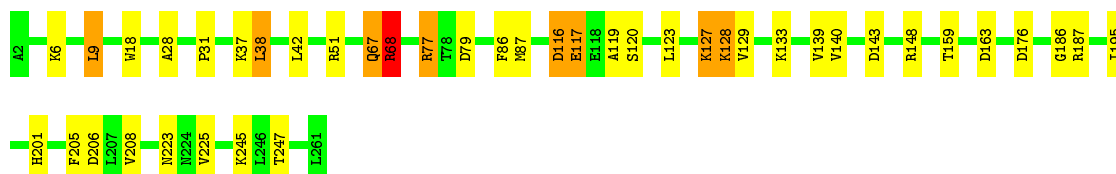
• Molecule 51: KLLA0D08305p

Chain D: 85% 12% •



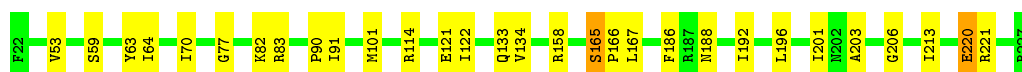
• Molecule 52: 40S ribosomal protein S4

Chain E: 84% 13% •



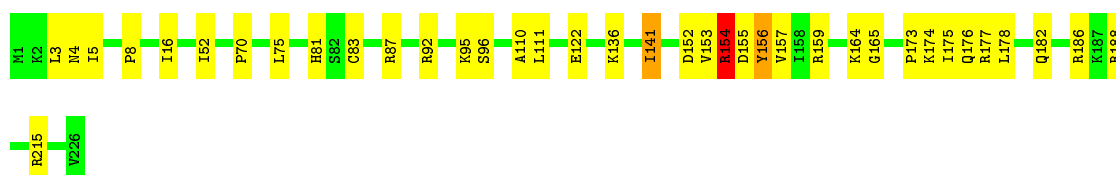
• Molecule 53: KLLA0D10659p

Chain F: 85% 14% •

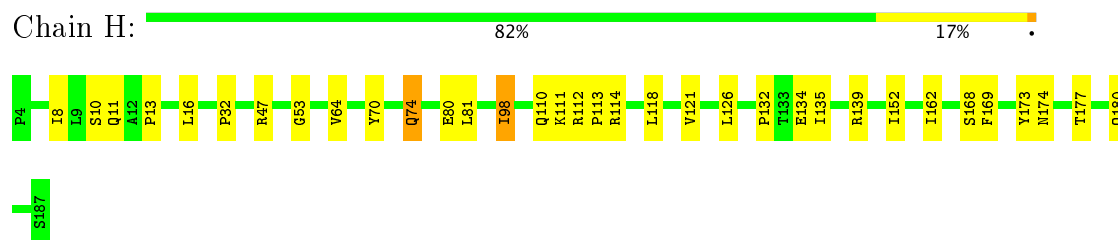


• Molecule 54: 40S ribosomal protein S6

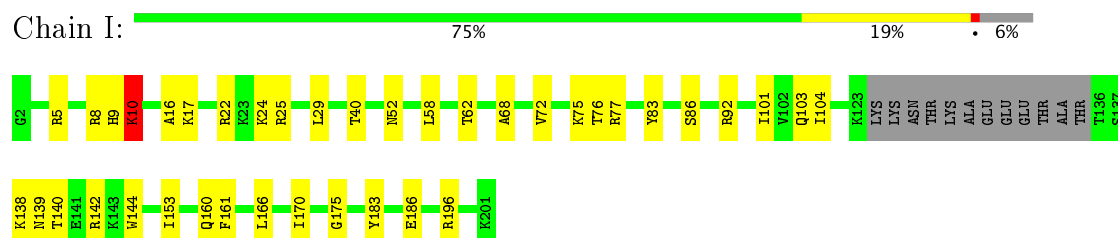
Chain G: 83% 15% •



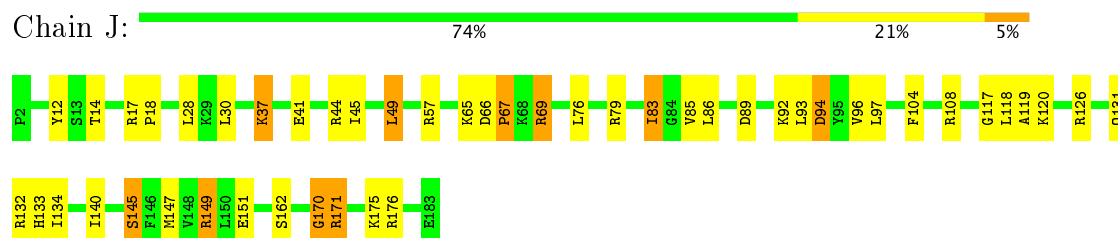
• Molecule 55: KLLA0C13519p



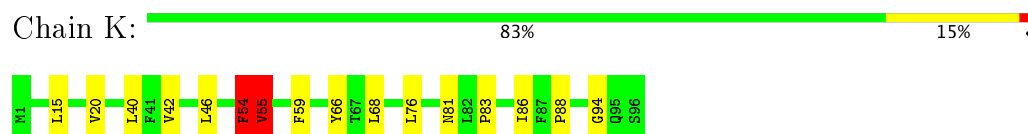
- Molecule 56: 40S ribosomal protein S8



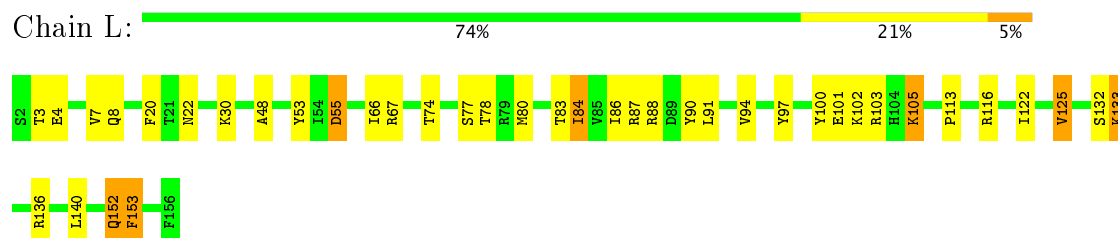
- Molecule 57: KLLA0E23673p



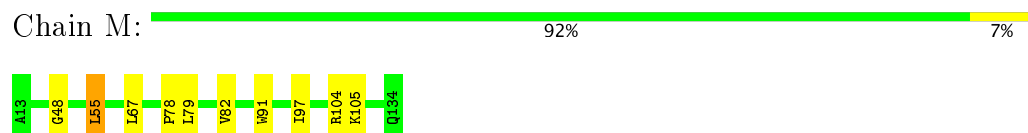
- Molecule 58: KLLA0B08173p



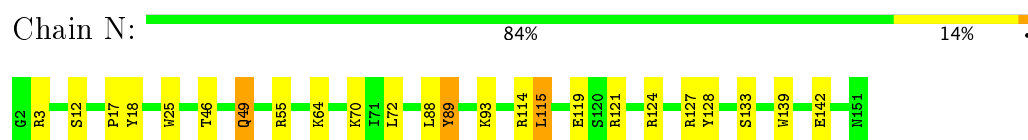
- Molecule 59: KLLA0A10483p



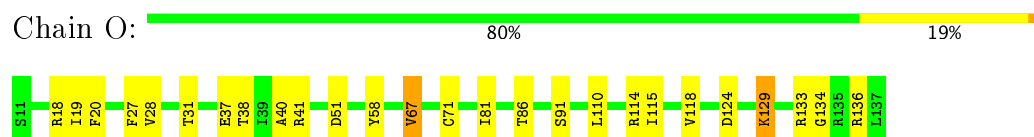
- Molecule 60: 40S ribosomal protein S12



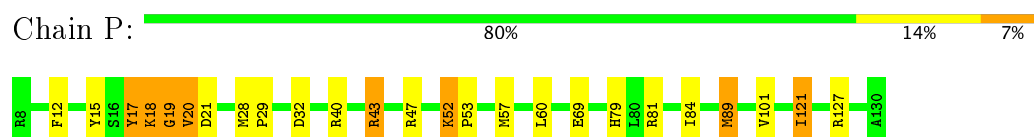
- Molecule 61: KLLA0F18040p



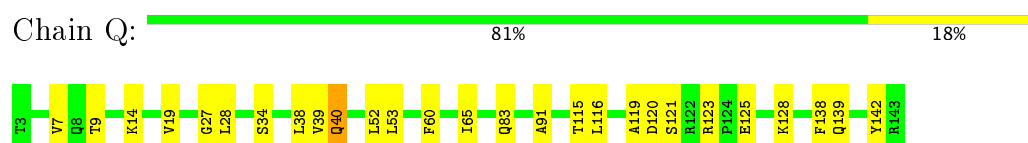
- Molecule 62: 40S ribosomal protein S14



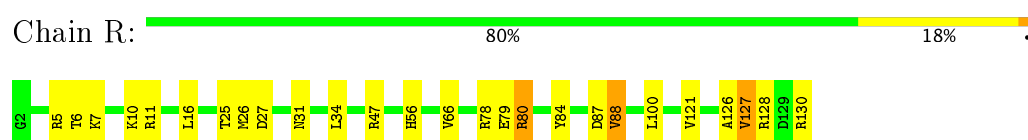
- Molecule 63: KLLA0F07843p



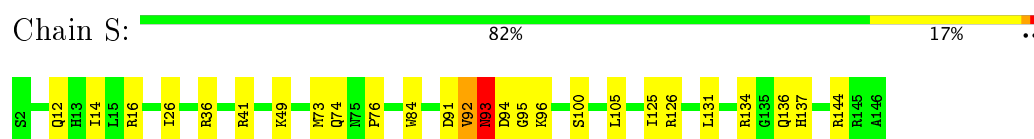
- Molecule 64: 40S ribosomal protein S16



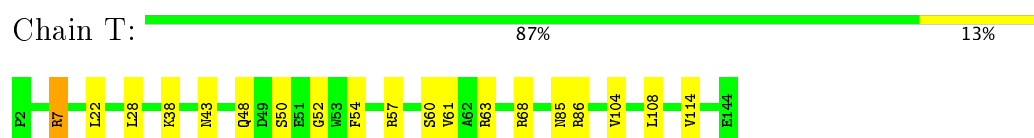
- Molecule 65: KLLA0B01474p




- Molecule 66: KLLA0B01562p



- Molecule 67: KLLA0A07194p



- Molecule 68: KLLA0F25542p

Chain U:  89% 11%



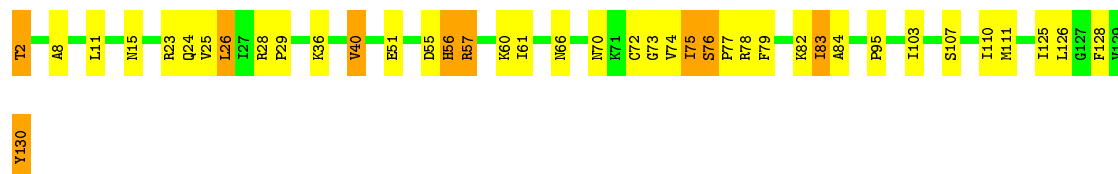
- Molecule 69: 40S ribosomal protein S21

Chain V:  76% 22% .



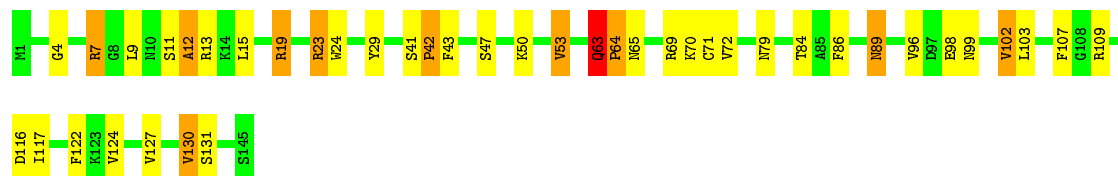
- Molecule 70: 40S ribosomal protein S22

Chain W:  69% 24% 7%




- Molecule 71: RPS23

Chain X:  71% 21% 7% .




- Molecule 72: 40S ribosomal protein S24

Chain Y:  82% 16%



- Molecule 73: KLLA0B06182p

Chain Z:  90% 9%



- Molecule 74: KLLA0D05115p

Chain a:  72% 23% . .



- Molecule 75: 40S ribosomal protein S27

Chain b: 91% 7% .



- Molecule 76: 40S ribosomal protein S28

Chain c: 95% 5%



- Molecule 77: 40S ribosomal protein S29

Chain d: 94% 6%



- Molecule 78: KLLA0C04809p

Chain e: 89% 11%



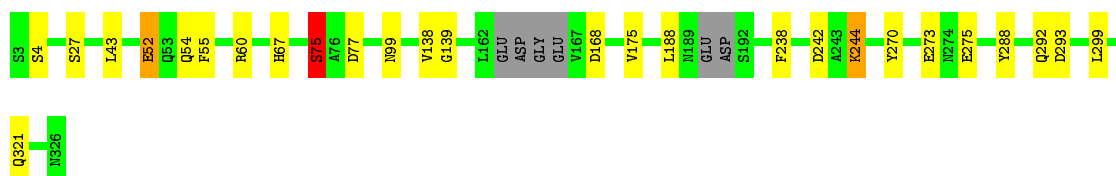
- Molecule 79: Ubiquitin-40S ribosomal protein S27a

Chain f: 78% 17% .



- Molecule 80: KLLA0E12277p

Chain g: 90% 7% ..



- Molecule 81: 18S ribosomal RNA

Chain 2: 34% 51% 13% ..

| | | | | | | | | | | | | | | |
|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| G1127 | U1056 | G390 | U856 | G786 | U715 | G642 | G573 | U507 | G431 | U367 | U291 | A216 | A146 | U1 |
| U1128 | A991 | A992 | G857 | A787 | C716 | G647 | C574 | G508 | C432 | A368 | U292 | A217 | U147 | A2 |
| G1129 | C1058 | G932 | A858 | A788 | U718 | U648 | G575 | G509 | G433 | A369 | C293 | A218 | U148 | U3 |
| A1130 | G933 | A932 | A859 | U789 | U719 | U649 | G576 | A510 | A434 | G370 | A294 | A219 | U149 | U4 |
| A1131 | U1059 | A994 | A860 | A790 | G720 | U650 | U577 | A511 | A435 | G371 | A295 | A220 | U150 | U5 |
| A1132 | U1060 | | A861 | U791 | U721 | G652 | A578 | U512 | A436 | G372 | A296 | A221 | U151 | U6 |
| A1136 | G1063 | | A862 | A792 | U722 | G653 | A579 | G513 | U438 | U373 | A297 | A222 | U152 | U7 |
| A1137 | U1070 | G937 | A863 | U793 | G723 | G654 | U580 | A514 | U439 | G374 | A298 | A223 | U153 | U8 |
| G1138 | A1002 | A938 | A864 | U794 | G724 | G655 | U581 | G515 | A440 | A375 | U301 | A224 | U154 | U9 |
| G1139 | U1003 | A939 | | A795 | G725 | G656 | C582 | G516 | C441 | | U302 | A225 | U155 | G10 |
| G1140 | A1004 | A940 | | | G726 | U657 | C583 | C518 | C442 | | U303 | U226 | U156 | A11 |
| A1141 | G1073 | G941 | | | G727 | G657 | A584 | A519 | C443 | | C304 | U227 | U157 | A12 |
| A1142 | U1074 | C942 | | | C727 | C | G585 | | C444 | | C305 | U228 | U158 | C13 |
| G1145 | A1075 | U943 | | | C731 | G | C586 | G522 | A445 | | G306 | U229 | U159 | C14 |
| A1146 | C1076 | U944 | | | G732 | A | | U523 | C447 | | U307 | U230 | U160 | U15 |
| C1147 | U1008 | U945 | | | G733 | C | G591 | U524 | | | C308 | U231 | C159 | G16 |
| G1148 | A1080 | U946 | | | A734 | U | U592 | A525 | A451 | | C309 | C232 | A84 | C17 |
| G1149 | C1081 | U947 | | | C735 | U | A593 | A526 | U452 | | C310 | C233 | A85 | C18 |
| G1150 | A1082 | C948 | | | U736 | U | G594 | U527 | U453 | | U311 | C234 | G162 | A19 |
| G1153 | A1083 | C949 | | | A737 | A | C595 | C530 | C454 | | U312 | C235 | C165 | G20 |
| G1154 | A1086 | C950 | | | G738 | U | G596 | U531 | A455 | | C313 | U240 | U166 | U21 |
| | A1087 | C951 | | | A813 | G | | U532 | A456 | | A314 | U241 | A167 | A22 |
| G1157 | A1090 | U952 | | | G814 | U | A600 | U533 | G458 | | A315 | U242 | A168 | C23 |
| C1158 | A1091 | U953 | | | G815 | C | U602 | A534 | A459 | | U319 | U243 | U169 | C25 |
| A1159 | A1092 | U954 | | | G816 | G | U603 | C535 | G460 | | C320 | C249 | A170 | A26 |
| A1162 | G1093 | U955 | | | G817 | C | A604 | G536 | A463 | | G321 | U253 | U173 | U29 |
| G1163 | U1094 | U956 | | | C818 | G | A605 | U537 | A464 | | A322 | U254 | C175 | G30 |
| | G1095 | U957 | | | G819 | C | G606 | G538 | A465 | | U323 | A255 | U176 | C31 |
| G1166 | U1096 | U958 | | | U820 | A | U607 | U539 | A466 | | G325 | C256 | U177 | U32 |
| A1170 | A1097 | U959 | | | U821 | C | G608 | A540 | A469 | | U326 | C257 | U178 | U33 |
| G1171 | G1099 | U960 | | | G822 | G | G609 | A541 | | | A327 | U258 | A179 | G34 |
| C1172 | A1100 | U961 | | | G823 | G | U610 | C542 | A473 | | G328 | U259 | A180 | C38 |
| C1173 | U1101 | U962 | | | U824 | C | C613 | A543 | A474 | | A330 | U260 | C186 | A39 |
| U1174 | G1102 | U963 | | | A760 | A | G614 | C544 | A475 | | U331 | A264 | U187 | A40 |
| G1175 | U1031 | U964 | | | G761 | A684 | G615 | U546 | A476 | | U332 | A265 | U188 | A41 |
| C1176 | C1032 | U965 | | | U762 | | | G547 | C478 | | G333 | U266 | G185 | G42 |
| G1177 | A1033 | U966 | | | G763 | | A618 | G548 | G479 | | U334 | C267 | G186 | U45 |
| G1178 | G1034 | U967 | | | U764 | | A619 | | A480 | | G335 | C268 | A187 | A46 |
| C1179 | A1035 | U968 | | | G765 | | A620 | C553 | C483 | | C337 | C269 | C190 | A47 |
| | G1036 | U969 | | | U766 | | A621 | U554 | | | U338 | G273 | U191 | G48 |
| G1184 | U1037 | U970 | | | G767 | | A622 | A555 | G487 | | C342 | C274 | U192 | G49 |
| U1185 | A1038 | U971 | | | U768 | | G623 | G556 | | | U349 | C275 | U193 | C50 |
| A1188 | G1039 | U972 | | | A769 | | U624 | U557 | | | U350 | U276 | G194 | C51 |
| A1193 | U1040 | U973 | | | A770 | | U625 | C558 | C490 | | U351 | U277 | G195 | U52 |
| G1194 | A1041 | U974 | | | A771 | | U626 | U559 | A491 | | A351 | U278 | G196 | G53 |
| C1195 | G1042 | U975 | | | A772 | | G627 | G560 | U492 | | U356 | U279 | A197 | U54 |
| G1197 | U1043 | U976 | | | A773 | | U628 | G561 | U493 | | G356 | G280 | G198 | C54 |
| G1198 | A1044 | U977 | | | G775 | | A629 | U562 | C494 | | U357 | C281 | U199 | G57 |
| G1199 | G1045 | U978 | | | G776 | | G630 | G563 | | | A358 | U282 | U200 | U58 |
| G1200 | U1046 | U979 | | | G777 | | U631 | C564 | G497 | | C359 | U283 | G203 | A61 |
| G1201 | A1047 | U980 | | | G778 | | A634 | C565 | U498 | | U360 | G284 | U204 | A62 |
| A1202 | G1048 | U981 | | | A779 | | | A566 | C499 | | A361 | C285 | A205 | G63 |
| | U1049 | U982 | | | U780 | | U637 | G567 | U500 | | G362 | G286 | U206 | U64 |
| | A1123 | U983 | | | A781 | | U638 | A568 | U503 | | G363 | A287 | U207 | G65 |
| | A1124 | U984 | | | G782 | | U639 | G570 | A504 | | G364 | U288 | U208 | U66 |
| | G1202 | U985 | | | U783 | | U640 | C571 | A505 | | A365 | G289 | A209 | A65 |
| A1202 | G1206 | U986 | | | U784 | | A713 | C572 | U506 | | C366 | G290 | U210 | A67 |
| | | C989 | | | G785 | | C714 | | | | A367 | | | |




4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 37844 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, 6EM, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # $ Z > 2$ | RMSZ | # $ Z > 2$ |
| 1 | 5 | 0.51 | 19/78233 (0.0%) | 0.81 | 74/121966 (0.1%) |
| 10 | GG | 0.44 | 0/1846 | 0.69 | 0/2486 |
| 11 | HH | 0.43 | 0/1547 | 0.73 | 0/2083 |
| 12 | II | 0.48 | 0/1725 | 0.74 | 0/2310 |
| 13 | JJ | 0.40 | 0/1370 | 0.71 | 0/1835 |
| 14 | LL | 0.48 | 0/1607 | 0.78 | 0/2156 |
| 15 | MM | 0.44 | 0/1060 | 0.74 | 0/1430 |
| 16 | NN | 0.69 | 0/1746 | 0.88 | 0/2339 |
| 17 | OO | 0.72 | 0/1602 | 0.79 | 0/2151 |
| 18 | PP | 0.58 | 0/1455 | 0.79 | 1/1952 (0.1%) |
| 19 | QQ | 0.48 | 0/1469 | 0.81 | 1/1970 (0.1%) |
| 2 | 7 | 0.38 | 0/2883 | 0.71 | 0/4491 |
| 20 | RR | 0.47 | 0/1539 | 0.78 | 0/2047 |
| 21 | SS | 0.52 | 0/1452 | 0.76 | 0/1956 |
| 22 | TT | 0.51 | 0/1286 | 0.76 | 0/1722 |
| 23 | UU | 0.38 | 0/824 | 0.59 | 0/1113 |
| 24 | VV | 0.58 | 0/991 | 0.84 | 0/1331 |
| 25 | WW | 0.51 | 0/528 | 0.74 | 0/703 |
| 26 | XX | 0.47 | 0/979 | 0.75 | 0/1320 |
| 27 | YY | 0.45 | 0/1003 | 0.78 | 0/1339 |
| 28 | ZZ | 0.46 | 0/1114 | 0.75 | 0/1493 |
| 29 | aa | 0.57 | 0/1186 | 0.83 | 1/1590 (0.1%) |
| 3 | 8 | 0.47 | 0/3714 | 0.78 | 2/5781 (0.0%) |
| 30 | bb | 0.43 | 0/468 | 0.68 | 0/621 |
| 31 | cc | 0.45 | 0/748 | 0.68 | 0/1005 |
| 32 | dd | 0.48 | 0/885 | 0.72 | 0/1186 |
| 33 | ee | 0.59 | 0/998 | 0.78 | 0/1332 |
| 34 | ff | 0.64 | 0/855 | 0.83 | 0/1150 |
| 35 | gg | 0.52 | 0/961 | 0.84 | 0/1281 |
| 36 | hh | 0.43 | 0/970 | 0.71 | 0/1291 |
| 37 | ii | 0.43 | 0/773 | 0.79 | 0/1029 |
| 38 | jj | 0.73 | 0/690 | 0.93 | 2/913 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 39 | kk | 0.47 | 0/626 | 0.82 | 0/835 |
| 4 | AA | 0.62 | 0/1926 | 0.92 | 3/2588 (0.1%) |
| 40 | ll | 0.60 | 0/435 | 0.93 | 1/577 (0.2%) |
| 41 | mm | 0.49 | 0/416 | 0.78 | 0/552 |
| 42 | nn | 0.43 | 0/234 | 0.91 | 0/300 |
| 43 | oo | 0.47 | 0/825 | 0.81 | 0/1086 |
| 44 | pp | 0.62 | 0/667 | 0.95 | 1/891 (0.1%) |
| 45 | qq | 0.60 | 4/1748 (0.2%) | 0.83 | 7/2350 (0.3%) |
| 46 | rr | 0.41 | 0/1535 | 0.67 | 0/2077 |
| 48 | A | 0.40 | 0/1656 | 0.71 | 0/2264 |
| 49 | B | 0.40 | 0/1747 | 0.69 | 0/2353 |
| 5 | BB | 0.61 | 0/3136 | 0.86 | 1/4225 (0.0%) |
| 50 | C | 0.45 | 0/1659 | 0.81 | 4/2252 (0.2%) |
| 51 | D | 0.37 | 0/1769 | 0.61 | 0/2378 |
| 52 | E | 0.42 | 0/2122 | 0.75 | 0/2861 |
| 53 | F | 0.37 | 0/1628 | 0.65 | 2/2198 (0.1%) |
| 54 | G | 0.45 | 2/1835 (0.1%) | 0.70 | 0/2451 |
| 55 | H | 0.37 | 0/1507 | 0.66 | 0/2028 |
| 56 | I | 0.42 | 0/1519 | 0.73 | 0/2033 |
| 57 | J | 0.56 | 2/1495 (0.1%) | 0.82 | 2/2001 (0.1%) |
| 58 | K | 0.39 | 0/831 | 0.57 | 1/1123 (0.1%) |
| 59 | L | 0.43 | 0/1276 | 0.76 | 0/1718 |
| 6 | CC | 0.54 | 0/2780 | 0.83 | 2/3760 (0.1%) |
| 60 | M | 0.40 | 0/929 | 0.59 | 0/1255 |
| 61 | N | 0.41 | 0/1210 | 0.71 | 0/1628 |
| 62 | O | 0.42 | 0/953 | 0.75 | 1/1279 (0.1%) |
| 63 | P | 0.50 | 1/1000 (0.1%) | 0.71 | 1/1343 (0.1%) |
| 64 | Q | 0.38 | 0/1125 | 0.61 | 0/1510 |
| 65 | R | 0.37 | 0/1042 | 0.70 | 0/1399 |
| 66 | S | 0.43 | 0/1212 | 0.69 | 1/1629 (0.1%) |
| 67 | T | 0.36 | 0/1129 | 0.60 | 0/1520 |
| 68 | U | 0.35 | 0/857 | 0.60 | 0/1158 |
| 69 | V | 0.40 | 0/696 | 0.68 | 0/938 |
| 7 | DD | 0.43 | 0/2436 | 0.71 | 0/3292 |
| 70 | W | 0.51 | 0/1039 | 0.81 | 0/1399 |
| 71 | X | 0.48 | 0/1145 | 0.83 | 1/1526 (0.1%) |
| 72 | Y | 0.39 | 0/1075 | 0.65 | 0/1433 |
| 73 | Z | 0.39 | 0/567 | 0.63 | 0/762 |
| 74 | a | 0.48 | 0/810 | 0.92 | 1/1084 (0.1%) |
| 75 | b | 0.36 | 0/627 | 0.68 | 0/847 |
| 76 | c | 0.36 | 0/496 | 0.69 | 0/666 |
| 77 | d | 0.38 | 0/457 | 0.61 | 0/607 |
| 78 | e | 0.36 | 0/450 | 0.65 | 0/599 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 79 | f | 0.43 | 0/562 | 0.65 | 0/751 |
| 8 | EE | 0.43 | 0/1322 | 0.79 | 2/1776 (0.1%) |
| 80 | g | 0.36 | 0/2521 | 0.58 | 0/3431 |
| 81 | 2 | 0.36 | 6/42269 (0.0%) | 0.78 | 20/65862 (0.0%) |
| 82 | 4 | 0.30 | 0/4407 | 0.84 | 6/6849 (0.1%) |
| 83 | 1 | 0.42 | 1/6540 (0.0%) | 0.80 | 10/8853 (0.1%) |
| 9 | FF | 0.58 | 0/1810 | 0.80 | 0/2440 |
| All | All | 0.47 | 35/230565 (0.0%) | 0.78 | 148/338109 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 5 | 0 | 6 |
| 14 | LL | 0 | 1 |
| 21 | SS | 0 | 1 |
| 27 | YY | 0 | 1 |
| 28 | ZZ | 0 | 1 |
| 29 | aa | 0 | 1 |
| 34 | ff | 0 | 1 |
| 35 | gg | 0 | 2 |
| 4 | AA | 0 | 2 |
| 44 | pp | 0 | 3 |
| 45 | qq | 0 | 3 |
| 46 | rr | 0 | 1 |
| 48 | A | 0 | 2 |
| 49 | B | 0 | 1 |
| 5 | BB | 0 | 1 |
| 50 | C | 0 | 3 |
| 51 | D | 0 | 1 |
| 52 | E | 0 | 3 |
| 53 | F | 0 | 1 |
| 58 | K | 0 | 1 |
| 59 | L | 0 | 1 |
| 6 | CC | 0 | 3 |
| 62 | O | 0 | 1 |
| 63 | P | 0 | 1 |
| 64 | Q | 0 | 1 |
| 65 | R | 0 | 2 |
| 69 | V | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7 | DD | 0 | 1 |
| 70 | W | 0 | 2 |
| 71 | X | 0 | 1 |
| 74 | a | 0 | 4 |
| 79 | f | 0 | 2 |
| 8 | EE | 0 | 3 |
| 80 | g | 0 | 1 |
| 82 | 4 | 1 | 0 |
| 83 | 1 | 0 | 16 |
| 9 | FF | 0 | 2 |
| All | All | 1 | 78 |

All (35) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1 | 5 | 2219 | G | O3'-P | -16.66 | 1.41 | 1.61 |
| 57 | J | 170 | GLY | CA-C | 11.07 | 1.69 | 1.51 |
| 81 | 2 | 510 | A | O3'-P | 9.75 | 1.72 | 1.61 |
| 45 | qq | 123 | LEU | N-CA | 7.99 | 1.62 | 1.46 |
| 1 | 5 | 2239 | A | O3'-P | -7.87 | 1.51 | 1.61 |
| 57 | J | 170 | GLY | N-CA | 7.70 | 1.57 | 1.46 |
| 81 | 2 | 511 | A | O5'-C5' | 7.35 | 1.56 | 1.44 |
| 1 | 5 | 2219 | G | C3'-O3' | -7.15 | 1.32 | 1.42 |
| 54 | G | 154 | ARG | CA-C | 6.45 | 1.69 | 1.52 |
| 1 | 5 | 627 | C | O3'-P | -6.36 | 1.53 | 1.61 |
| 45 | qq | 119 | GLN | CA-C | 6.21 | 1.69 | 1.52 |
| 1 | 5 | 2782 | G | O3'-P | -6.15 | 1.53 | 1.61 |
| 1 | 5 | 29 | C | O3'-P | -6.04 | 1.53 | 1.61 |
| 1 | 5 | 2479 | U | O3'-P | -5.98 | 1.53 | 1.61 |
| 81 | 2 | 991 | A | O3'-P | -5.90 | 1.54 | 1.61 |
| 81 | 2 | 77 | U | O3'-P | 5.70 | 1.68 | 1.61 |
| 1 | 5 | 918 | G | O3'-P | -5.63 | 1.54 | 1.61 |
| 1 | 5 | 2377 | U | O3'-P | -5.62 | 1.54 | 1.61 |
| 1 | 5 | 2691 | U | O3'-P | -5.51 | 1.54 | 1.61 |
| 1 | 5 | 3015 | U | O3'-P | -5.48 | 1.54 | 1.61 |
| 81 | 2 | 940 | A | O3'-P | -5.46 | 1.54 | 1.61 |
| 1 | 5 | 2217 | C | O3'-P | -5.45 | 1.54 | 1.61 |
| 1 | 5 | 1129 | A | O3'-P | -5.44 | 1.54 | 1.61 |
| 1 | 5 | 2958 | G | O3'-P | -5.39 | 1.54 | 1.61 |
| 63 | P | 19 | GLY | N-CA | 5.35 | 1.54 | 1.46 |
| 1 | 5 | 1378 | A | O3'-P | -5.34 | 1.54 | 1.61 |
| 1 | 5 | 899 | C | O3'-P | -5.33 | 1.54 | 1.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 45 | qq | 120 | VAL | N-CA | 5.32 | 1.56 | 1.46 |
| 1 | 5 | 2328 | C | O3'-P | -5.29 | 1.54 | 1.61 |
| 83 | 1 | 585 | ARG | N-CA | -5.22 | 1.35 | 1.46 |
| 54 | G | 154 | ARG | N-CA | 5.20 | 1.56 | 1.46 |
| 1 | 5 | 1581 | A | O3'-P | -5.07 | 1.55 | 1.61 |
| 81 | 2 | 1790 | G | O3'-P | -5.06 | 1.55 | 1.61 |
| 45 | qq | 120 | VAL | CA-CB | 5.06 | 1.65 | 1.54 |
| 1 | 5 | 3025 | U | O3'-P | -5.06 | 1.55 | 1.61 |

All (148) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 83 | 1 | 581 | ASN | N-CA-CB | 18.89 | 144.59 | 110.60 |
| 1 | 5 | 2049 | G | N9-C1'-C2' | -12.44 | 97.83 | 114.00 |
| 81 | 2 | 511 | A | P-O5'-C5' | 10.73 | 138.07 | 120.90 |
| 83 | 1 | 580 | PRO | N-CA-C | 10.27 | 138.81 | 112.10 |
| 81 | 2 | 23 | G | N9-C1'-C2' | -10.23 | 100.70 | 114.00 |
| 45 | qq | 124 | LEU | CA-CB-CG | 9.47 | 137.08 | 115.30 |
| 82 | 4 | 6121 | A | C4'-C3'-O3' | 9.31 | 131.63 | 113.00 |
| 1 | 5 | 2219 | G | C8-N9-C1' | -8.92 | 115.40 | 127.00 |
| 82 | 4 | 6201 | C | N1-C1'-C2' | -8.87 | 102.24 | 112.00 |
| 45 | qq | 123 | LEU | CA-CB-CG | 8.84 | 135.62 | 115.30 |
| 1 | 5 | 2151 | A | O5'-P-OP1 | -8.52 | 98.03 | 105.70 |
| 83 | 1 | 581 | ASN | N-CA-C | -8.35 | 88.46 | 111.00 |
| 81 | 2 | 931 | U | C2'-C3'-O3' | -8.25 | 91.35 | 109.50 |
| 1 | 5 | 3207 | G | C2'-C3'-O3' | 8.02 | 127.15 | 109.50 |
| 1 | 5 | 2630 | G | C2'-C3'-O3' | 7.89 | 126.85 | 109.50 |
| 81 | 2 | 1628 | U | C4'-C3'-O3' | 7.86 | 128.73 | 113.00 |
| 1 | 5 | 596 | U | C2'-C3'-O3' | 7.83 | 126.73 | 109.50 |
| 1 | 5 | 2218 | G | O4'-C1'-N9 | 7.82 | 114.45 | 108.20 |
| 1 | 5 | 2218 | G | C1'-C2'-O2' | 7.77 | 133.92 | 110.60 |
| 1 | 5 | 297 | G | C2'-C3'-O3' | 7.74 | 126.53 | 109.50 |
| 81 | 2 | 78 | A | C4'-C3'-O3' | 7.70 | 128.41 | 113.00 |
| 1 | 5 | 1196 | A | C2'-C3'-O3' | 7.44 | 125.86 | 109.50 |
| 3 | 8 | 8 | C | N1-C1'-C2' | -7.42 | 103.84 | 112.00 |
| 1 | 5 | 2053 | C | N1-C1'-C2' | -7.42 | 103.84 | 112.00 |
| 1 | 5 | 65 | A | C2'-C3'-O3' | 7.35 | 125.67 | 109.50 |
| 4 | AA | 174 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 1 | 5 | 2285 | G | N9-C1'-C2' | -7.26 | 104.01 | 112.00 |
| 1 | 5 | 2239 | A | C5'-C4'-O4' | 7.24 | 117.79 | 109.10 |
| 1 | 5 | 2219 | G | P-O3'-C3' | -7.21 | 111.04 | 119.70 |
| 1 | 5 | 3055 | A | C4-N9-C1' | 7.19 | 139.23 | 126.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81 | 2 | 11 | A | N9-C1'-C2' | -7.17 | 104.11 | 112.00 |
| 1 | 5 | 3055 | A | C8-N9-C1' | -7.05 | 115.01 | 127.70 |
| 1 | 5 | 957 | U | N1-C1'-C2' | 6.88 | 122.94 | 114.00 |
| 1 | 5 | 1209 | C | C2'-C3'-O3' | 6.86 | 124.68 | 113.70 |
| 1 | 5 | 2049 | G | C4'-C3'-O3' | 6.78 | 126.56 | 113.00 |
| 50 | C | 149 | TRP | CA-CB-CG | 6.74 | 126.50 | 113.70 |
| 83 | 1 | 381 | TYR | N-CA-C | 6.60 | 128.82 | 111.00 |
| 81 | 2 | 9 | U | N1-C1'-C2' | -6.59 | 104.75 | 112.00 |
| 1 | 5 | 2050 | A | C4'-C3'-O3' | -6.58 | 95.59 | 109.40 |
| 1 | 5 | 2946 | U | N1-C1'-C2' | 6.55 | 122.52 | 114.00 |
| 81 | 2 | 78 | A | C5'-C4'-C3' | 6.55 | 126.48 | 116.00 |
| 83 | 1 | 380 | LEU | N-CA-C | 6.55 | 128.68 | 111.00 |
| 8 | EE | 114 | ARG | N-CA-C | 6.49 | 128.52 | 111.00 |
| 1 | 5 | 2062 | A | N9-C1'-C2' | 6.39 | 122.31 | 114.00 |
| 8 | EE | 13 | VAL | C-N-CD | -6.39 | 106.54 | 120.60 |
| 83 | 1 | 585 | ARG | CA-C-N | -6.35 | 103.22 | 117.20 |
| 45 | qq | 122 | ARG | N-CA-C | 6.30 | 128.02 | 111.00 |
| 1 | 5 | 1452 | A | C2'-C3'-O3' | -6.18 | 95.90 | 109.50 |
| 71 | X | 7 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 81 | 2 | 911 | U | N1-C1'-C2' | 6.16 | 122.01 | 114.00 |
| 82 | 4 | 6039 | A | C4'-C3'-O3' | 6.16 | 125.33 | 113.00 |
| 1 | 5 | 1255 | C | C2'-C3'-O3' | 6.16 | 123.55 | 113.70 |
| 1 | 5 | 3257 | A | C2'-C3'-O3' | 6.14 | 123.52 | 113.70 |
| 1 | 5 | 2229 | U | O5'-P-OP2 | -6.10 | 100.21 | 105.70 |
| 1 | 5 | 2922 | U | C2'-C3'-O3' | 6.08 | 123.43 | 113.70 |
| 1 | 5 | 2050 | A | C5'-C4'-O4' | 6.08 | 116.39 | 109.10 |
| 57 | J | 170 | GLY | N-CA-C | 6.07 | 128.28 | 113.10 |
| 1 | 5 | 2219 | G | O4'-C1'-N9 | 6.04 | 113.03 | 108.20 |
| 1 | 5 | 298 | U | C2'-C3'-O3' | 6.03 | 123.35 | 113.70 |
| 53 | F | 220 | GLU | N-CA-C | 6.00 | 127.21 | 111.00 |
| 81 | 2 | 1534 | G | C2'-C3'-O3' | 5.99 | 123.29 | 113.70 |
| 1 | 5 | 3325 | U | C2'-C3'-O3' | 5.95 | 123.21 | 113.70 |
| 38 | jj | 21 | ARG | NE-CZ-NH2 | -5.92 | 117.34 | 120.30 |
| 58 | K | 55 | VAL | N-CA-C | -5.92 | 95.03 | 111.00 |
| 1 | 5 | 2481 | C | C5'-C4'-O4' | 5.91 | 116.19 | 109.10 |
| 82 | 4 | 6134 | C | N1-C1'-C2' | -5.88 | 105.53 | 112.00 |
| 50 | C | 149 | TRP | N-CA-CB | 5.84 | 121.12 | 110.60 |
| 1 | 5 | 707 | A | C2'-C3'-O3' | 5.73 | 122.87 | 113.70 |
| 1 | 5 | 1452 | A | N9-C1'-C2' | 5.73 | 121.44 | 114.00 |
| 1 | 5 | 1531 | G | C2'-C3'-O3' | 5.72 | 122.85 | 113.70 |
| 1 | 5 | 1608 | C | O5'-P-OP2 | -5.71 | 100.56 | 105.70 |
| 29 | aa | 21 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81 | 2 | 1501 | A | C2'-C3'-O3' | 5.68 | 122.79 | 113.70 |
| 81 | 2 | 22 | A | N9-C1'-C2' | -5.67 | 105.76 | 112.00 |
| 1 | 5 | 2032 | U | C2'-C3'-O3' | 5.64 | 122.72 | 113.70 |
| 81 | 2 | 10 | G | N9-C1'-C2' | -5.63 | 105.80 | 112.00 |
| 1 | 5 | 2218 | G | P-O5'-C5' | -5.63 | 111.89 | 120.90 |
| 81 | 2 | 963 | U | C2'-C3'-O3' | 5.61 | 122.68 | 113.70 |
| 1 | 5 | 336 | A | C8-N9-C1' | -5.58 | 117.65 | 127.70 |
| 1 | 5 | 336 | A | N9-C1'-C2' | 5.58 | 121.25 | 114.00 |
| 44 | pp | 47 | VAL | CB-CA-C | 5.57 | 121.99 | 111.40 |
| 4 | AA | 207 | VAL | CB-CA-C | -5.57 | 100.81 | 111.40 |
| 18 | PP | 69 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 53 | F | 165 | SER | C-N-CD | -5.56 | 108.38 | 120.60 |
| 1 | 5 | 307 | A | N9-C1'-C2' | 5.56 | 121.22 | 114.00 |
| 1 | 5 | 282 | G | C2'-C3'-O3' | 5.55 | 122.57 | 113.70 |
| 45 | qq | 123 | LEU | CB-CG-CD1 | 5.54 | 120.42 | 111.00 |
| 1 | 5 | 336 | A | C4-N9-C1' | 5.54 | 136.27 | 126.30 |
| 1 | 5 | 1337 | A | O5'-P-OP2 | -5.53 | 100.73 | 105.70 |
| 1 | 5 | 2238 | U | C4'-C3'-O3' | 5.52 | 124.04 | 113.00 |
| 81 | 2 | 828 | A | C2'-C3'-O3' | 5.48 | 122.47 | 113.70 |
| 1 | 5 | 2217 | C | O3'-P-O5' | -5.47 | 93.60 | 104.00 |
| 83 | 1 | 579 | SER | C-N-CD | 5.47 | 139.89 | 128.40 |
| 82 | 4 | 6039 | A | N9-C1'-C2' | -5.46 | 105.99 | 112.00 |
| 1 | 5 | 2529 | C | N1-C1'-C2' | 5.44 | 121.08 | 114.00 |
| 1 | 5 | 887 | G | C4'-C3'-O3' | 5.43 | 123.86 | 113.00 |
| 5 | BB | 159 | ARG | NE-CZ-NH2 | -5.42 | 117.59 | 120.30 |
| 50 | C | 174 | LEU | C-N-CA | 5.39 | 135.18 | 121.70 |
| 3 | 8 | 7 | U | N1-C1'-C2' | -5.38 | 106.08 | 112.00 |
| 45 | qq | 125 | GLY | N-CA-C | 5.37 | 126.53 | 113.10 |
| 83 | 1 | 585 | ARG | C-N-CA | 5.37 | 135.13 | 121.70 |
| 1 | 5 | 2510 | U | N1-C1'-C2' | 5.37 | 120.98 | 114.00 |
| 6 | CC | 348 | LYS | N-CA-C | 5.37 | 125.50 | 111.00 |
| 1 | 5 | 1052 | U | C2'-C3'-O3' | 5.37 | 122.29 | 113.70 |
| 1 | 5 | 1155 | A | C2'-C3'-O3' | 5.36 | 122.27 | 113.70 |
| 1 | 5 | 96 | G | O5'-P-OP2 | -5.34 | 100.90 | 105.70 |
| 1 | 5 | 2217 | C | P-O3'-C3' | -5.31 | 113.33 | 119.70 |
| 4 | AA | 204 | MET | CA-CB-CG | 5.31 | 122.33 | 113.30 |
| 1 | 5 | 1926 | U | C4'-C3'-O3' | 5.30 | 123.60 | 113.00 |
| 66 | S | 93 | ASN | N-CA-C | 5.29 | 125.29 | 111.00 |
| 1 | 5 | 1863 | U | C2'-C3'-O3' | 5.29 | 122.16 | 113.70 |
| 1 | 5 | 1600 | C | C2'-C3'-O3' | 5.28 | 122.15 | 113.70 |
| 62 | O | 133 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | 5 | 364 | G | C2'-C3'-O3' | 5.27 | 122.14 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | 5 | 2241 | G | N9-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 1 | 5 | 2054 | U | C4'-C3'-O3' | 5.27 | 123.54 | 113.00 |
| 6 | CC | 202 | ARG | NE-CZ-NH2 | 5.27 | 122.93 | 120.30 |
| 83 | 1 | 208 | THR | C-N-CA | 5.24 | 134.81 | 121.70 |
| 1 | 5 | 238 | A | C2'-C3'-O3' | 5.24 | 122.08 | 113.70 |
| 45 | qq | 175 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | 5 | 3135 | A | C2'-C3'-O3' | 5.23 | 122.06 | 113.70 |
| 81 | 2 | 990 | G | C4'-C3'-O3' | 5.21 | 123.42 | 113.00 |
| 1 | 5 | 2341 | A | C2'-C3'-O3' | 5.19 | 122.00 | 113.70 |
| 1 | 5 | 2372 | G | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 1 | 5 | 1337 | A | O5'-P-OP1 | 5.17 | 116.91 | 110.70 |
| 81 | 2 | 78 | A | P-O5'-C5' | 5.16 | 129.16 | 120.90 |
| 1 | 5 | 1278 | G | C2'-C3'-O3' | 5.16 | 121.95 | 113.70 |
| 1 | 5 | 78 | U | O4'-C4'-C3' | -5.14 | 98.86 | 104.00 |
| 57 | J | 49 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 63 | P | 20 | VAL | N-CA-C | 5.11 | 124.80 | 111.00 |
| 82 | 4 | 6121 | A | C2'-C3'-O3' | -5.10 | 98.28 | 109.50 |
| 1 | 5 | 2784 | G | C2'-C3'-O3' | -5.09 | 98.30 | 109.50 |
| 45 | qq | 119 | GLN | CA-CB-CG | 5.08 | 124.57 | 113.40 |
| 1 | 5 | 987 | C | C2'-C3'-O3' | 5.07 | 121.81 | 113.70 |
| 1 | 5 | 2239 | A | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 19 | QQ | 178 | ARG | NE-CZ-NH1 | -5.07 | 117.77 | 120.30 |
| 81 | 2 | 279 | U | C2'-C3'-O3' | 5.06 | 121.80 | 113.70 |
| 50 | C | 82 | LYS | C-N-CA | 5.06 | 134.35 | 121.70 |
| 1 | 5 | 2285 | G | C2'-C3'-O3' | -5.06 | 98.37 | 109.50 |
| 1 | 5 | 2238 | U | N1-C1'-C2' | -5.05 | 106.44 | 112.00 |
| 1 | 5 | 886 | A | O5'-P-OP1 | -5.04 | 101.17 | 105.70 |
| 81 | 2 | 469 | A | C2'-C3'-O3' | 5.04 | 121.76 | 113.70 |
| 74 | a | 83 | ILE | CB-CA-C | -5.04 | 101.53 | 111.60 |
| 81 | 2 | 77 | U | P-O3'-C3' | 5.04 | 125.74 | 119.70 |
| 1 | 5 | 844 | C | C4'-C3'-O3' | 5.02 | 123.04 | 113.00 |
| 38 | jj | 11 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 83 | 1 | 161 | ASP | N-CA-C | 5.01 | 124.54 | 111.00 |
| 40 | ll | 45 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 82 | 4 | 6205 | DA | C4' |

All (78) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 83 | 1 | 463 | LEU | Peptide |
| 83 | 1 | 464 | LEU | Peptide |
| 83 | 1 | 576 | LEU | Peptide |
| 83 | 1 | 577 | SER | Peptide |
| 83 | 1 | 669 | TRP | Peptide |
| 83 | 1 | 680 | GLU | Peptide |
| 83 | 1 | 681 | MET | Peptide |
| 83 | 1 | 682 | ARG | Peptide |
| 83 | 1 | 683 | SER | Peptide |
| 83 | 1 | 684 | VAL | Peptide |
| 83 | 1 | 693 | LEU | Peptide |
| 83 | 1 | 694 | HIS | Peptide |
| 83 | 1 | 695 | ALA | Peptide |
| 83 | 1 | 696 | ASP | Peptide |
| 83 | 1 | 697 | ALA | Peptide |
| 83 | 1 | 707 | PRO | Peptide |
| 1 | 5 | 1178 | G | Sidechain |
| 1 | 5 | 2049 | G | Sidechain |
| 1 | 5 | 2218 | G | Sidechain |
| 1 | 5 | 2219 | G | Sidechain |
| 1 | 5 | 2285 | G | Sidechain |
| 1 | 5 | 2629 | G | Sidechain |
| 48 | A | 164 | ASN | Peptide |
| 48 | A | 33 | GLN | Peptide |
| 4 | AA | 196 | TRP | Peptide |
| 4 | AA | 33 | ASP | Peptide |
| 49 | B | 35 | PRO | Peptide |
| 5 | BB | 331 | THR | Peptide |
| 50 | C | 111 | ASP | Peptide |
| 50 | C | 148 | TYR | Peptide |
| 50 | C | 177 | ALA | Peptide |
| 6 | CC | 148 | ILE | Peptide |
| 6 | CC | 80 | GLY | Peptide |
| 6 | CC | 82 | THR | Peptide |
| 51 | D | 176 | LEU | Peptide |
| 7 | DD | 3 | PHE | Peptide |
| 52 | E | 116 | ASP | Peptide |
| 52 | E | 128 | LYS | Peptide |
| 52 | E | 67 | GLN | Peptide |
| 8 | EE | 110 | SER | Peptide |
| 8 | EE | 112 | LYS | Mainchain |
| 8 | EE | 65 | GLY | Peptide |
| 53 | F | 165 | SER | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 9 | FF | 112 | THR | Peptide |
| 9 | FF | 220 | PHE | Peptide |
| 58 | K | 54 | PHE | Peptide |
| 59 | L | 152 | GLN | Peptide |
| 14 | LL | 74 | GLY | Peptide |
| 62 | O | 129 | LYS | Peptide |
| 63 | P | 15 | TYR | Peptide |
| 64 | Q | 40 | GLN | Peptide |
| 65 | R | 78 | ARG | Peptide |
| 65 | R | 79 | GLU | Peptide |
| 21 | SS | 12 | ARG | Peptide |
| 69 | V | 13 | VAL | Peptide |
| 70 | W | 56 | HIS | Peptide |
| 70 | W | 75 | ILE | Peptide |
| 71 | X | 63 | GLN | Peptide |
| 27 | YY | 55 | GLU | Peptide |
| 28 | ZZ | 88 | ASP | Peptide |
| 74 | a | 34 | LYS | Peptide |
| 74 | a | 49 | ALA | Peptide |
| 74 | a | 83 | ILE | Peptide |
| 74 | a | 9 | GLY | Peptide |
| 29 | aa | 112 | VAL | Peptide |
| 79 | f | 102 | VAL | Peptide |
| 79 | f | 103 | LEU | Peptide |
| 34 | ff | 103 | TYR | Peptide |
| 80 | g | 75 | SER | Peptide |
| 35 | gg | 26 | PRO | Peptide |
| 35 | gg | 8 | ARG | Peptide |
| 44 | pp | 37 | TYR | Peptide |
| 44 | pp | 55 | TRP | Peptide |
| 44 | pp | 56 | SER | Peptide |
| 45 | qq | 117 | ILE | Peptide |
| 45 | qq | 120 | VAL | Peptide |
| 45 | qq | 123 | LEU | Peptide |
| 46 | rr | 20 | TYR | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 5 | 69896 | 0 | 35118 | 1365 | 0 |
| 2 | 7 | 2579 | 0 | 1304 | 23 | 0 |
| 3 | 8 | 3326 | 0 | 1680 | 65 | 0 |
| 4 | AA | 1892 | 0 | 1954 | 47 | 0 |
| 5 | BB | 3064 | 0 | 3140 | 80 | 0 |
| 6 | CC | 2731 | 0 | 2842 | 84 | 0 |
| 7 | DD | 2384 | 0 | 2337 | 27 | 0 |
| 8 | EE | 1300 | 0 | 1393 | 25 | 0 |
| 9 | FF | 1774 | 0 | 1832 | 31 | 0 |
| 10 | GG | 1817 | 0 | 1927 | 32 | 0 |
| 11 | HH | 1528 | 0 | 1596 | 19 | 0 |
| 12 | II | 1690 | 0 | 1729 | 20 | 0 |
| 13 | JJ | 1349 | 0 | 1382 | 8 | 0 |
| 14 | LL | 1581 | 0 | 1661 | 37 | 0 |
| 15 | MM | 1045 | 0 | 1126 | 11 | 0 |
| 16 | NN | 1709 | 0 | 1763 | 20 | 0 |
| 17 | OO | 1571 | 0 | 1663 | 417 | 0 |
| 18 | PP | 1432 | 0 | 1465 | 27 | 0 |
| 19 | QQ | 1444 | 0 | 1541 | 27 | 0 |
| 20 | RR | 1522 | 0 | 1624 | 20 | 0 |
| 21 | SS | 1416 | 0 | 1461 | 15 | 0 |
| 22 | TT | 1262 | 0 | 1309 | 19 | 0 |
| 23 | UU | 807 | 0 | 821 | 5 | 0 |
| 24 | VV | 976 | 0 | 1021 | 28 | 0 |
| 25 | WW | 515 | 0 | 532 | 2 | 0 |
| 26 | XX | 964 | 0 | 1031 | 7 | 0 |
| 27 | YY | 992 | 0 | 1070 | 12 | 0 |
| 28 | ZZ | 1089 | 0 | 1150 | 23 | 0 |
| 29 | aa | 1156 | 0 | 1206 | 0 | 0 |
| 30 | bb | 458 | 0 | 486 | 0 | 0 |
| 31 | cc | 740 | 0 | 792 | 0 | 0 |
| 32 | dd | 869 | 0 | 920 | 0 | 0 |
| 33 | ee | 980 | 0 | 1048 | 0 | 0 |
| 34 | ff | 837 | 0 | 861 | 0 | 0 |
| 35 | gg | 951 | 0 | 1036 | 0 | 0 |
| 36 | hh | 961 | 0 | 1062 | 0 | 0 |
| 37 | ii | 766 | 0 | 840 | 0 | 0 |
| 38 | jj | 675 | 0 | 679 | 0 | 0 |
| 39 | kk | 619 | 0 | 675 | 0 | 0 |
| 40 | ll | 428 | 0 | 464 | 0 | 0 |
| 41 | mm | 410 | 0 | 446 | 0 | 0 |
| 42 | nn | 233 | 0 | 284 | 0 | 0 |
| 43 | oo | 814 | 0 | 875 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44 | pp | 660 | 0 | 690 | 0 | 0 |
| 45 | qq | 1721 | 0 | 1820 | 0 | 0 |
| 46 | rr | 1508 | 0 | 1542 | 0 | 0 |
| 47 | KK | 735 | 0 | 177 | 0 | 0 |
| 48 | A | 1616 | 0 | 1636 | 22 | 0 |
| 49 | B | 1722 | 0 | 1793 | 17 | 0 |
| 50 | C | 1629 | 0 | 1710 | 19 | 0 |
| 51 | D | 1744 | 0 | 1826 | 8 | 0 |
| 52 | E | 2078 | 0 | 2157 | 9 | 0 |
| 53 | F | 1609 | 0 | 1679 | 7 | 0 |
| 54 | G | 1812 | 0 | 1911 | 35 | 0 |
| 55 | H | 1483 | 0 | 1579 | 8 | 0 |
| 56 | I | 1493 | 0 | 1515 | 12 | 0 |
| 57 | J | 1471 | 0 | 1553 | 36 | 0 |
| 58 | K | 809 | 0 | 810 | 6 | 0 |
| 59 | L | 1248 | 0 | 1311 | 18 | 0 |
| 60 | M | 922 | 0 | 953 | 1 | 0 |
| 61 | N | 1187 | 0 | 1251 | 8 | 0 |
| 62 | O | 942 | 0 | 979 | 8 | 0 |
| 63 | P | 980 | 0 | 1029 | 12 | 0 |
| 64 | Q | 1105 | 0 | 1170 | 9 | 0 |
| 65 | R | 1031 | 0 | 1082 | 7 | 0 |
| 66 | S | 1193 | 0 | 1217 | 9 | 0 |
| 67 | T | 1110 | 0 | 1124 | 7 | 0 |
| 68 | U | 845 | 0 | 913 | 3 | 0 |
| 69 | V | 687 | 0 | 682 | 7 | 0 |
| 70 | W | 1021 | 0 | 1056 | 21 | 0 |
| 71 | X | 1127 | 0 | 1210 | 23 | 0 |
| 72 | Y | 1061 | 0 | 1111 | 7 | 0 |
| 73 | Z | 558 | 0 | 585 | 2 | 0 |
| 74 | a | 798 | 0 | 854 | 0 | 0 |
| 75 | b | 617 | 0 | 643 | 0 | 0 |
| 76 | c | 494 | 0 | 534 | 0 | 0 |
| 77 | d | 446 | 0 | 436 | 0 | 0 |
| 78 | e | 443 | 0 | 481 | 0 | 0 |
| 79 | f | 549 | 0 | 564 | 0 | 0 |
| 80 | g | 2466 | 0 | 2406 | 0 | 0 |
| 81 | 2 | 37797 | 0 | 19015 | 680 | 0 |
| 82 | 4 | 3950 | 0 | 1982 | 120 | 0 |
| 83 | 1 | 6421 | 0 | 6490 | 456 | 0 |
| 84 | 1 | 1 | 0 | 0 | 0 | 0 |
| 84 | 2 | 75 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 84 | 5 | 2 | 0 | 0 | 0 | 0 |
| 84 | N | 1 | 0 | 0 | 0 | 0 |
| 84 | f | 1 | 0 | 0 | 0 | 0 |
| 85 | a | 1 | 0 | 0 | 0 | 0 |
| 85 | b | 1 | 0 | 0 | 0 | 0 |
| 85 | f | 1 | 0 | 0 | 0 | 0 |
| 85 | jj | 1 | 0 | 0 | 0 | 0 |
| 85 | mm | 1 | 0 | 0 | 0 | 0 |
| 85 | oo | 1 | 0 | 0 | 0 | 0 |
| 86 | 1 | 32 | 0 | 14 | 1 | 0 |
| 87 | 1 | 10 | 0 | 0 | 2 | 0 |
| All | All | 215768 | 0 | 160636 | 3749 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (3749) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 81:2:884:G:H2' | 81:2:885:U:C1' | 1.20 | 1.64 |
| 83:1:698:ILE:HG22 | 83:1:699:HIS:CD2 | 1.33 | 1.58 |
| 1:5:2217:C:C3' | 1:5:2218:G:H5' | 1.16 | 1.57 |
| 83:1:576:LEU:HD21 | 83:1:587:TYR:CD1 | 1.36 | 1.57 |
| 1:5:2217:C:H3' | 1:5:2218:G:C5' | 1.12 | 1.54 |
| 1:5:2167:A:C5 | 1:5:2238:U:C4 | 1.97 | 1.52 |
| 83:1:587:TYR:CE2 | 83:1:690:ASP:N | 1.77 | 1.50 |
| 8:EE:13:VAL:HG22 | 8:EE:14:PRO:CD | 1.48 | 1.42 |
| 1:5:2167:A:C4 | 1:5:2238:U:C5 | 2.05 | 1.42 |
| 1:5:1923:G:N2 | 1:5:1925:G:C8 | 1.76 | 1.41 |
| 83:1:698:ILE:CG2 | 83:1:699:HIS:HD2 | 1.33 | 1.41 |
| 81:2:884:G:C2' | 81:2:885:U:H1' | 1.49 | 1.40 |
| 83:1:587:TYR:CD2 | 83:1:690:ASP:N | 1.90 | 1.38 |
| 8:EE:13:VAL:CG2 | 8:EE:14:PRO:HD2 | 1.52 | 1.37 |
| 83:1:587:TYR:HE2 | 83:1:691:VAL:N | 1.25 | 1.35 |
| 83:1:576:LEU:CD2 | 83:1:587:TYR:CD1 | 2.11 | 1.34 |
| 83:1:806:SER:OG | 83:1:815:ALA:HB3 | 1.25 | 1.33 |
| 17:OO:168[A]:TYR:O | 17:OO:168[A]:TYR:CD1 | 1.80 | 1.33 |
| 17:OO:34[A]:ILE:CG2 | 17:OO:35[A]:VAL:H | 1.39 | 1.32 |
| 83:1:584:ASN:HB2 | 83:1:692:THR:O | 1.29 | 1.32 |
| 57:J:14:THR:HG21 | 81:2:23:G:OP1 | 1.24 | 1.31 |
| 81:2:884:G:C2' | 81:2:885:U:C1' | 2.01 | 1.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 83:1:586:ILE:HD11 | 83:1:708:THR:OG1 | 1.13 | 1.30 |
| 1:5:2234:C:O2' | 1:5:2235:U:H5' | 1.22 | 1.28 |
| 17:OO:86[A]:ARG:HB2 | 17:OO:100[A]:LEU:CD1 | 1.63 | 1.27 |
| 17:OO:20[A]:LEU:O | 17:OO:20[A]:LEU:CD1 | 1.82 | 1.27 |
| 17:OO:86[A]:ARG:HD3 | 17:OO:86[A]:ARG:O | 1.35 | 1.27 |
| 83:1:806:SER:OG | 83:1:815:ALA:CB | 1.83 | 1.27 |
| 81:2:886:A:C2 | 81:2:925:A:C2 | 2.22 | 1.27 |
| 83:1:580:PRO:HD2 | 83:1:583:HIS:CE1 | 1.70 | 1.27 |
| 83:1:702:GLY:CA | 83:1:706:ILE:HD12 | 1.65 | 1.26 |
| 1:5:2481:C:H2' | 1:5:2482:U:C6 | 1.71 | 1.26 |
| 8:EE:128:GLU:O | 8:EE:129:ILE:CG1 | 1.83 | 1.25 |
| 81:2:1292:U:O4 | 81:2:1321:A:N1 | 1.68 | 1.25 |
| 17:OO:192[A]:GLU:O | 17:OO:194[A]:LEU:N | 1.66 | 1.25 |
| 83:1:581:ASN:H | 83:1:583:HIS:CD2 | 1.55 | 1.25 |
| 81:2:480:A:N1 | 81:2:506:U:C4 | 2.05 | 1.25 |
| 83:1:580:PRO:HG2 | 83:1:583:HIS:NE2 | 1.51 | 1.25 |
| 83:1:576:LEU:CD2 | 83:1:587:TYR:HD1 | 1.45 | 1.24 |
| 83:1:698:ILE:HB | 83:1:699:HIS:C | 1.56 | 1.24 |
| 1:5:2481:C:OP2 | 10:GG:244:LYS:NZ | 1.69 | 1.24 |
| 83:1:587:TYR:CE2 | 83:1:691:VAL:N | 2.04 | 1.24 |
| 83:1:133:GLU:OE2 | 83:1:136:CYS:CB | 1.87 | 1.23 |
| 82:4:6199:A:O2' | 82:4:6200:A:H5' | 1.34 | 1.23 |
| 83:1:702:GLY:HA2 | 83:1:706:ILE:CD1 | 1.68 | 1.23 |
| 83:1:695:ALA:O | 83:1:700:ARG:NH1 | 1.72 | 1.22 |
| 1:5:1925:G:H21 | 1:5:2056:C:C3' | 1.51 | 1.22 |
| 83:1:380:LEU:HD13 | 83:1:400:VAL:CG2 | 1.68 | 1.21 |
| 1:5:2167:A:C4 | 1:5:2238:U:C6 | 2.28 | 1.21 |
| 83:1:586:ILE:CD1 | 83:1:708:THR:OG1 | 1.86 | 1.21 |
| 1:5:2481:C:O2' | 1:5:2482:U:O4' | 1.57 | 1.21 |
| 1:5:78:U:O4 | 1:5:325:A:N1 | 1.72 | 1.21 |
| 1:5:1925:G:N3 | 1:5:2056:C:C2 | 2.09 | 1.21 |
| 17:OO:107[A]:GLU:CD | 17:OO:107[A]:GLU:H | 1.40 | 1.20 |
| 1:5:2167:A:C6 | 1:5:2238:U:C4 | 2.29 | 1.20 |
| 14:LL:2:ALA:O | 14:LL:3:ILE:HG22 | 1.04 | 1.20 |
| 1:5:2167:A:C6 | 1:5:2238:U:O4 | 1.94 | 1.20 |
| 1:5:2234:C:O2' | 1:5:2235:U:C5' | 1.87 | 1.20 |
| 1:5:2167:A:C2 | 1:5:2238:U:C5 | 2.29 | 1.19 |
| 83:1:638:PRO:HD2 | 83:1:681:MET:CE | 1.72 | 1.19 |
| 17:OO:20[A]:LEU:O | 17:OO:20[A]:LEU:HD12 | 1.33 | 1.18 |
| 1:5:1923:G:N2 | 1:5:1925:G:H8 | 1.16 | 1.18 |
| 81:2:480:A:N1 | 81:2:506:U:O4 | 1.77 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 81:2:886:A:H2 | 81:2:925:A:C2 | 1.58 | 1.18 |
| 83:1:705:ILE:HA | 83:1:708:THR:CG2 | 1.74 | 1.18 |
| 1:5:529:U:N3 | 1:5:532:A:N6 | 1.91 | 1.17 |
| 83:1:133:GLU:OE2 | 83:1:136:CYS:SG | 2.01 | 1.17 |
| 14:LL:2:ALA:O | 14:LL:3:ILE:CG2 | 1.92 | 1.17 |
| 1:5:2167:A:C5 | 1:5:2238:U:C5 | 2.27 | 1.17 |
| 83:1:380:LEU:HD13 | 83:1:400:VAL:HG22 | 1.20 | 1.17 |
| 17:OO:65[A]:PHE:CD1 | 17:OO:65[A]:PHE:O | 1.97 | 1.17 |
| 1:5:2481:C:O5' | 10:GG:244:LYS:HE2 | 1.43 | 1.16 |
| 83:1:698:ILE:HD11 | 83:1:700:ARG:NE | 1.39 | 1.16 |
| 83:1:695:ALA:C | 83:1:700:ARG:NH1 | 1.98 | 1.16 |
| 17:OO:107[A]:GLU:O | 17:OO:107[A]:GLU:OE2 | 1.63 | 1.16 |
| 83:1:698:ILE:CG2 | 83:1:699:HIS:CD2 | 2.13 | 1.16 |
| 1:5:1924:C:N4 | 1:5:2055:G:O6 | 1.78 | 1.16 |
| 17:OO:168[A]:TYR:O | 17:OO:168[A]:TYR:CG | 1.97 | 1.16 |
| 1:5:1924:C:O2' | 1:5:1926:U:OP2 | 1.59 | 1.15 |
| 17:OO:111[A]:PRO:HB2 | 17:OO:112[A]:PRO:CD | 1.76 | 1.15 |
| 83:1:580:PRO:HD2 | 83:1:583:HIS:NE2 | 1.62 | 1.15 |
| 83:1:705:ILE:HA | 83:1:708:THR:HG22 | 1.28 | 1.15 |
| 17:OO:104[A]:LYS:O | 17:OO:105[A]:VAL:HG23 | 1.43 | 1.15 |
| 1:5:1925:G:N2 | 1:5:2056:C:H3' | 1.60 | 1.15 |
| 57:J:14:THR:HG21 | 81:2:23:G:P | 1.84 | 1.15 |
| 83:1:587:TYR:CE2 | 83:1:690:ASP:CA | 2.29 | 1.14 |
| 17:OO:86[A]:ARG:CB | 17:OO:100[A]:LEU:HD11 | 1.76 | 1.14 |
| 83:1:580:PRO:CG | 83:1:583:HIS:NE2 | 2.09 | 1.14 |
| 17:OO:104[A]:LYS:O | 17:OO:105[A]:VAL:CG2 | 1.96 | 1.14 |
| 83:1:204:PRO:HG2 | 83:1:245:TRP:CZ2 | 1.82 | 1.14 |
| 83:1:581:ASN:N | 83:1:583:HIS:HD2 | 1.45 | 1.14 |
| 1:5:2167:A:N3 | 1:5:2238:U:C5 | 2.16 | 1.14 |
| 17:OO:35[A]:VAL:HG13 | 17:OO:35[A]:VAL:O | 1.45 | 1.14 |
| 17:OO:44[A]:ILE:HD11 | 17:OO:139[A]:LEU:HD11 | 1.25 | 1.13 |
| 81:2:928:A:H2' | 81:2:929:A:H5' | 1.25 | 1.13 |
| 1:5:1159:U:O4 | 1:5:1288:A:N1 | 1.81 | 1.12 |
| 17:OO:107[A]:GLU:OE2 | 17:OO:107[A]:GLU:N | 1.81 | 1.12 |
| 83:1:580:PRO:HD2 | 83:1:583:HIS:CD2 | 1.83 | 1.12 |
| 17:OO:86[A]:ARG:HB2 | 17:OO:100[A]:LEU:HD11 | 1.17 | 1.12 |
| 81:2:884:G:C2' | 81:2:885:U:O4' | 1.96 | 1.12 |
| 1:5:2481:C:P | 10:GG:244:LYS:HZ1 | 1.73 | 1.12 |
| 1:5:2167:A:C2 | 1:5:2238:U:H5 | 1.64 | 1.12 |
| 1:5:1924:C:N3 | 1:5:2055:G:N1 | 1.97 | 1.11 |
| 1:5:2239:A:H2' | 1:5:2240:A:C8 | 1.85 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|-----------------------|--------------------------|-------------------|
| 81:2:1439:C:O2' | 81:2:1445:C:N4 | 1.82 | 1.11 |
| 83:1:584:ASN:HD22 | 83:1:693:LEU:HD13 | 1.16 | 1.10 |
| 82:4:6120:U:H1' | 82:4:6127:C:H5'' | 1.33 | 1.10 |
| 83:1:587:TYR:CD2 | 83:1:689:LEU:C | 2.21 | 1.10 |
| 1:5:2237:U:O4 | 1:5:2241:G:N1 | 1.84 | 1.10 |
| 17:OO:31[A]:GLY:O | 17:OO:32[A]:GLN:O | 1.67 | 1.10 |
| 83:1:702:GLY:HA2 | 83:1:706:ILE:HD12 | 1.19 | 1.10 |
| 1:5:2218:G:H1' | 1:5:2219:G:H5' | 1.20 | 1.10 |
| 8:EE:128:GLU:O | 8:EE:129:ILE:HG13 | 0.93 | 1.10 |
| 83:1:580:PRO:CD | 83:1:583:HIS:NE2 | 2.15 | 1.09 |
| 83:1:379:MET:SD | 83:1:380:LEU:HD22 | 1.93 | 1.09 |
| 57:J:14:THR:CG2 | 81:2:23:G:OP1 | 2.00 | 1.09 |
| 17:OO:114[A]:ASP:HA | 17:OO:118[A]:ARG:HH12 | 1.17 | 1.09 |
| 14:LL:5:LYS:H | 14:LL:5:LYS:HD2 | 1.18 | 1.08 |
| 1:5:1925:G:N2 | 1:5:2056:C:C3' | 2.15 | 1.08 |
| 81:2:928:A:C2' | 81:2:929:A:H5' | 1.84 | 1.08 |
| 17:OO:13[A]:LYS:HD2 | 17:OO:38[A]:ARG:NH2 | 1.68 | 1.08 |
| 83:1:584:ASN:CB | 83:1:692:THR:O | 2.01 | 1.07 |
| 83:1:380:LEU:CD1 | 83:1:400:VAL:HA | 1.84 | 1.07 |
| 17:OO:107[A]:GLU:CD | 17:OO:107[A]:GLU:N | 2.01 | 1.07 |
| 83:1:638:PRO:CD | 83:1:681:MET:CE | 2.33 | 1.07 |
| 83:1:698:ILE:HG22 | 83:1:699:HIS:CG | 1.88 | 1.07 |
| 1:5:2050:A:O2' | 1:5:2051:U:OP1 | 1.73 | 1.07 |
| 81:2:11:A:HO2' | 81:2:12:U:C5' | 1.67 | 1.06 |
| 17:OO:137[A]:THR:HG22 | 17:OO:138[A]:THR:H | 1.19 | 1.06 |
| 83:1:584:ASN:HD22 | 83:1:693:LEU:CD1 | 1.69 | 1.06 |
| 17:OO:34[A]:ILE:HG22 | 17:OO:35[A]:VAL:N | 1.46 | 1.06 |
| 83:1:580:PRO:CD | 83:1:583:HIS:CE1 | 2.38 | 1.06 |
| 17:OO:139[A]:LEU:O | 17:OO:141[A]:LYS:N | 1.89 | 1.06 |
| 83:1:693:LEU:HB3 | 83:1:695:ALA:HA | 1.09 | 1.06 |
| 1:5:2481:C:P | 10:GG:244:LYS:CE | 2.43 | 1.06 |
| 82:4:6181:C:H2' | 83:1:578:LYS:HZ3 | 1.14 | 1.05 |
| 81:2:1292:U:C4 | 81:2:1321:A:N1 | 2.24 | 1.05 |
| 1:5:2050:A:OP1 | 1:5:2051:U:C4 | 2.09 | 1.05 |
| 81:2:1267:G:N1 | 81:2:1439:C:N3 | 2.04 | 1.05 |
| 1:5:2055:G:C5 | 1:5:2056:C:N4 | 2.25 | 1.05 |
| 82:4:6199:A:C2' | 82:4:6200:A:H5' | 1.86 | 1.04 |
| 17:OO:20[A]:LEU:CG | 17:OO:20[A]:LEU:O | 2.05 | 1.04 |
| 83:1:638:PRO:CD | 83:1:681:MET:HE1 | 1.86 | 1.04 |
| 1:5:1925:G:N1 | 1:5:2056:C:C5 | 2.12 | 1.04 |
| 17:OO:91[A]:HIS:O | 17:OO:91[A]:HIS:CD2 | 2.11 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|--------------------|--------------------------|-------------------|
| 83:1:638:PRO:HD2 | 83:1:681:MET:HE1 | 1.06 | 1.03 |
| 17:OO:192[A]:GLU:C | 17:OO:194[A]:LEU:H | 1.58 | 1.03 |
| 81:2:885:U:C2' | 81:2:886:A:H5'' | 1.89 | 1.03 |
| 1:5:1928:A:C2 | 1:5:2053:C:H2' | 1.93 | 1.03 |
| 83:1:587:TYR:HE2 | 83:1:690:ASP:C | 1.62 | 1.03 |
| 81:2:884:G:H2' | 81:2:885:U:O4' | 1.53 | 1.03 |
| 83:1:16:VAL:HG11 | 83:1:372:CYS:SG | 1.98 | 1.03 |
| 83:1:380:LEU:HD12 | 83:1:399:ARG:C | 1.78 | 1.03 |
| 83:1:380:LEU:HD12 | 83:1:400:VAL:N | 1.74 | 1.02 |
| 83:1:684:VAL:HG12 | 83:1:686:VAL:HB | 1.40 | 1.02 |
| 1:5:2234:C:O2' | 1:5:2235:U:C4' | 2.08 | 1.02 |
| 17:OO:5[A]:GLU:N | 17:OO:5[A]:GLU:OE1 | 1.91 | 1.02 |
| 49:B:117:TRP:N | 81:2:931:U:OP2 | 1.93 | 1.02 |
| 17:OO:153[A]:VAL:HG12 | 17:OO:153[A]:VAL:O | 1.57 | 1.02 |
| 83:1:133:GLU:OE2 | 83:1:136:CYS:HB2 | 1.54 | 1.02 |
| 83:1:806:SER:HG | 83:1:815:ALA:CB | 1.64 | 1.02 |
| 81:2:628:U:N3 | 81:2:969:A:N6 | 2.06 | 1.02 |
| 1:5:2218:G:C6 | 1:5:2219:G:C4 | 2.48 | 1.02 |
| 57:J:170:GLY:HA3 | 81:2:510:A:H2' | 1.42 | 1.02 |
| 83:1:157:ILE:HD12 | 83:1:211:PHE:CE1 | 1.94 | 1.01 |
| 17:OO:34[A]:ILE:HG22 | 17:OO:35[A]:VAL:H | 0.86 | 1.01 |
| 1:5:2167:A:N3 | 1:5:2238:U:C6 | 2.28 | 1.01 |
| 82:4:6181:C:C2' | 83:1:578:LYS:HZ3 | 1.72 | 1.01 |
| 54:G:154:ARG:N | 81:2:78:A:O5' | 1.93 | 1.01 |
| 17:OO:176[A]:ASN:O | 17:OO:178[A]:VAL:N | 1.94 | 1.01 |
| 1:5:2218:G:N1 | 1:5:2219:G:C4 | 2.28 | 1.01 |
| 17:OO:197[A]:LEU:O | 17:OO:198[A]:GLY:C | 1.97 | 1.01 |
| 83:1:583:HIS:HE1 | 83:1:704:GLN:CD | 1.64 | 1.01 |
| 83:1:694:HIS:N | 83:1:700:ARG:HH12 | 1.58 | 1.00 |
| 17:OO:124[A]:ALA:O | 17:OO:125[A]:LEU:O | 1.79 | 1.00 |
| 83:1:589:LYS:HD3 | 83:1:685:ARG:HD2 | 1.39 | 1.00 |
| 1:5:2481:C:C2' | 1:5:2482:U:C6 | 2.45 | 1.00 |
| 1:5:2481:C:P | 10:GG:244:LYS:NZ | 2.33 | 1.00 |
| 1:5:2051:U:H4' | 1:5:2052:G:OP2 | 1.19 | 1.00 |
| 17:OO:158[A]:GLU:O | 17:OO:161[A]:ARG:N | 1.93 | 1.00 |
| 81:2:884:G:C3' | 81:2:885:U:O4' | 2.10 | 0.99 |
| 1:5:2237:U:N3 | 1:5:2241:G:O6 | 1.95 | 0.99 |
| 1:5:2480:A:H3' | 1:5:2481:C:C5' | 1.92 | 0.99 |
| 1:5:1925:G:H21 | 1:5:2056:C:C2' | 1.54 | 0.99 |
| 83:1:587:TYR:CE2 | 83:1:690:ASP:C | 2.36 | 0.99 |
| 83:1:702:GLY:HA2 | 83:1:706:ILE:CG1 | 1.93 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:2479:U:C2' | 1:5:2480:A:H5' | 1.92 | 0.99 |
| 1:5:601:A:H2' | 1:5:602:A:C8 | 1.98 | 0.98 |
| 81:2:11:A:O2' | 81:2:12:U:C5' | 2.09 | 0.98 |
| 1:5:2234:C:C2' | 1:5:2235:U:H5' | 1.94 | 0.98 |
| 57:J:170:GLY:HA3 | 81:2:510:A:C2' | 1.93 | 0.98 |
| 17:OO:176[A]:ASN:O | 17:OO:179[A]:VAL:N | 1.97 | 0.98 |
| 1:5:1925:G:O2' | 1:5:2056:C:O2 | 1.79 | 0.98 |
| 1:5:529:U:N3 | 1:5:532:A:C6 | 2.28 | 0.97 |
| 81:2:11:A:O2' | 81:2:12:U:H5' | 1.63 | 0.97 |
| 83:1:562:ALA:HB1 | 83:1:563:TYR:HA | 1.46 | 0.97 |
| 54:G:155:ASP:H | 81:2:78:A:C5' | 1.76 | 0.97 |
| 83:1:705:ILE:CA | 83:1:708:THR:HG22 | 1.95 | 0.97 |
| 1:5:2540:A:O2' | 1:5:2541:C:OP2 | 1.82 | 0.97 |
| 83:1:806:SER:HB2 | 83:1:813:SER:HB2 | 1.43 | 0.97 |
| 83:1:380:LEU:CD1 | 83:1:400:VAL:CA | 2.43 | 0.97 |
| 17:OO:65[A]:PHE:O | 17:OO:66[A]:ASN:HB2 | 1.65 | 0.96 |
| 83:1:380:LEU:HD13 | 83:1:400:VAL:HA | 1.45 | 0.96 |
| 81:2:884:G:O2' | 81:2:885:U:H1' | 1.65 | 0.96 |
| 17:OO:37[A]:VAL:O | 17:OO:38[A]:ARG:HB2 | 1.60 | 0.96 |
| 17:OO:9[A]:VAL:HG22 | 17:OO:35[A]:VAL:HG11 | 1.45 | 0.96 |
| 82:4:6121:A:H2' | 82:4:6121:A:N3 | 1.79 | 0.96 |
| 17:OO:120[A]:VAL:O | 17:OO:122[A]:PRO:HD3 | 1.65 | 0.96 |
| 1:5:2218:G:H5'' | 1:5:2242:G:N7 | 1.81 | 0.96 |
| 17:OO:192[A]:GLU:C | 17:OO:194[A]:LEU:N | 2.13 | 0.96 |
| 19:QQ:124:LEU:N | 82:4:6039:A:N3 | 121.63 | 0.96 |
| 82:4:6182:A:OP2 | 83:1:585:ARG:NH1 | 1.97 | 0.96 |
| 17:OO:40[A]:GLU:OE1 | 17:OO:108[A]:GLY:N | 1.98 | 0.96 |
| 83:1:698:ILE:HB | 83:1:700:ARG:N | 1.81 | 0.95 |
| 83:1:564:ARG:HD2 | 83:1:681:MET:CG | 1.96 | 0.95 |
| 1:5:2218:G:C6 | 1:5:2219:G:N3 | 2.34 | 0.95 |
| 17:OO:35[A]:VAL:O | 17:OO:35[A]:VAL:CG1 | 2.10 | 0.95 |
| 82:4:6181:C:H2' | 83:1:578:LYS:NZ | 1.81 | 0.95 |
| 83:1:698:ILE:HA | 83:1:699:HIS:HB3 | 1.44 | 0.95 |
| 17:OO:33[A]:LYS:O | 17:OO:34[A]:ILE:HG12 | 1.66 | 0.95 |
| 1:5:2051:U:C4' | 1:5:2052:G:OP2 | 2.13 | 0.95 |
| 83:1:703:GLY:N | 83:1:706:ILE:HB | 1.81 | 0.95 |
| 1:5:2167:A:N6 | 1:5:2238:U:O4 | 1.99 | 0.95 |
| 1:5:2541:C:OP1 | 28:ZZ:59:ALA:N | 2.00 | 0.95 |
| 83:1:380:LEU:CD1 | 83:1:400:VAL:CG2 | 2.44 | 0.94 |
| 8:EE:128:GLU:C | 8:EE:129:ILE:HG13 | 1.87 | 0.94 |
| 54:G:155:ASP:N | 81:2:78:A:O5' | 2.00 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 81:2:884:G:H2' | 81:2:885:U:H1' | 0.96 | 0.94 |
| 17:OO:122[A]:PRO:HA | 17:OO:125[A]:LEU:CD2 | 1.98 | 0.94 |
| 1:5:2049:G:N2 | 1:5:2052:G:O6 | 2.01 | 0.94 |
| 17:OO:193[A]:LYS:HA | 17:OO:193[A]:LYS:HE3 | 1.47 | 0.94 |
| 17:OO:194[A]:LEU:O | 17:OO:197[A]:LEU:N | 2.01 | 0.94 |
| 81:2:1752:A:O2' | 81:2:1753:A:OP1 | 1.85 | 0.94 |
| 83:1:698:ILE:CD1 | 83:1:700:ARG:NE | 2.22 | 0.94 |
| 6:CC:349:ILE:HG13 | 6:CC:350:LYS:CB | 1.98 | 0.94 |
| 83:1:703:GLY:O | 83:1:706:ILE:O | 1.85 | 0.94 |
| 83:1:580:PRO:HD2 | 83:1:583:HIS:CG | 2.02 | 0.93 |
| 1:5:1924:C:O2' | 1:5:1925:G:O5' | 1.85 | 0.93 |
| 17:OO:19[A]:ARG:O | 17:OO:21[A]:ALA:N | 2.01 | 0.93 |
| 17:OO:82[A]:TYR:O | 17:OO:82[A]:TYR:CD1 | 2.21 | 0.93 |
| 1:5:2480:A:P | 1:5:2481:C:H5'' | 2.07 | 0.93 |
| 83:1:698:ILE:HD11 | 83:1:700:ARG:HE | 1.17 | 0.93 |
| 81:2:1439:C:C2' | 81:2:1440:U:H5' | 1.98 | 0.93 |
| 82:4:6119:U:H5' | 82:4:6120:U:C5' | 1.98 | 0.93 |
| 1:5:2218:G:C2 | 1:5:2219:G:C8 | 2.56 | 0.93 |
| 1:5:1925:G:N2 | 1:5:2056:C:C2' | 2.27 | 0.93 |
| 1:5:2218:G:C4 | 1:5:2219:G:N9 | 2.37 | 0.93 |
| 17:OO:126[A]:ARG:HG3 | 17:OO:130[A]:LEU:HD22 | 1.51 | 0.93 |
| 17:OO:197[A]:LEU:O | 17:OO:199[A]:TYR:N | 2.01 | 0.92 |
| 83:1:583:HIS:CE1 | 83:1:704:GLN:NE2 | 2.37 | 0.92 |
| 83:1:133:GLU:CD | 83:1:136:CYS:HB2 | 1.90 | 0.92 |
| 83:1:463:LEU:HD11 | 83:1:467:GLY:HA3 | 1.48 | 0.92 |
| 83:1:380:LEU:HD13 | 83:1:400:VAL:CA | 1.97 | 0.92 |
| 1:5:1926:U:N3 | 1:5:1927:G:N7 | 2.18 | 0.92 |
| 17:OO:96[A]:GLY:O | 17:OO:99[A]:ALA:HB3 | 1.70 | 0.92 |
| 6:CC:349:ILE:HG13 | 6:CC:350:LYS:HG3 | 1.49 | 0.92 |
| 83:1:584:ASN:ND2 | 83:1:693:LEU:HD13 | 1.85 | 0.92 |
| 17:OO:141[A]:LYS:O | 17:OO:142[A]:LEU:C | 2.08 | 0.92 |
| 1:5:2167:A:C6 | 1:5:2238:U:C5 | 2.52 | 0.92 |
| 83:1:750:LYS:O | 83:1:751:ARG:HG3 | 1.69 | 0.92 |
| 81:2:8:U:O4 | 81:2:15:U:O4 | 1.88 | 0.92 |
| 17:OO:161[A]:ARG:O | 17:OO:163[A]:ALA:N | 2.01 | 0.92 |
| 83:1:579:SER:HB2 | 83:1:708:THR:HB | 1.52 | 0.91 |
| 82:4:6199:A:O2' | 82:4:6200:A:C5' | 2.17 | 0.91 |
| 1:5:2036:U:H2' | 1:5:2049:G:C6 | 2.05 | 0.91 |
| 1:5:2218:G:C5 | 1:5:2219:G:N9 | 2.38 | 0.91 |
| 17:OO:194[A]:LEU:O | 17:OO:196[A]:ALA:N | 2.03 | 0.91 |
| 17:OO:68[A]:THR:O | 17:OO:72[A]:PHE:HE1 | 1.52 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 83:1:380:LEU:CD1 | 83:1:400:VAL:HG22 | 1.99 | 0.91 |
| 17:OO:104[A]:LYS:C | 17:OO:105[A]:VAL:HG23 | 1.89 | 0.91 |
| 1:5:1925:G:O6 | 1:5:2057:A:C5 | 2.24 | 0.91 |
| 17:OO:111[A]:PRO:HB2 | 17:OO:112[A]:PRO:HD2 | 1.49 | 0.91 |
| 81:2:885:U:C3' | 81:2:886:A:H5'' | 2.01 | 0.91 |
| 1:5:2218:G:N3 | 1:5:2219:G:C8 | 2.39 | 0.91 |
| 17:OO:76[A]:ALA:O | 17:OO:79[A]:ARG:N | 2.04 | 0.91 |
| 1:5:2050:A:O2' | 1:5:2051:U:P | 2.28 | 0.90 |
| 1:5:2218:G:H2' | 1:5:2218:G:N3 | 1.87 | 0.90 |
| 1:5:2480:A:H5'' | 10:GG:248:ARG:CZ | 2.01 | 0.90 |
| 83:1:694:HIS:H | 83:1:700:ARG:NH1 | 1.68 | 0.90 |
| 82:4:6181:C:C3' | 83:1:578:LYS:HZ3 | 1.83 | 0.90 |
| 82:4:6181:C:H3' | 83:1:578:LYS:NZ | 1.86 | 0.90 |
| 17:OO:7[A]:VAL:CG1 | 17:OO:8[A]:VAL:N | 2.34 | 0.90 |
| 17:OO:145[A]:SER:O | 17:OO:146[A]:VAL:CG1 | 2.19 | 0.90 |
| 83:1:204:PRO:HG2 | 83:1:245:TRP:CE2 | 2.07 | 0.89 |
| 1:5:2480:A:H3' | 1:5:2481:C:H5'' | 1.52 | 0.89 |
| 6:CC:349:ILE:HG13 | 6:CC:350:LYS:CG | 2.02 | 0.89 |
| 83:1:694:HIS:CD2 | 83:1:700:ARG:HH22 | 1.88 | 0.89 |
| 1:5:2481:C:H2' | 1:5:2482:U:H6 | 1.32 | 0.89 |
| 17:OO:55[A]:TYR:O | 17:OO:57[A]:ASP:N | 2.05 | 0.89 |
| 17:OO:24[A]:VAL:HG22 | 17:OO:34[A]:ILE:HD12 | 1.53 | 0.89 |
| 17:OO:93[A]:THR:O | 17:OO:94[A]:ALA:C | 2.11 | 0.89 |
| 83:1:806:SER:HG | 83:1:815:ALA:HB3 | 0.74 | 0.88 |
| 17:OO:94[A]:ALA:O | 17:OO:96[A]:GLY:N | 2.06 | 0.88 |
| 81:2:1292:U:O4 | 81:2:1321:A:C2 | 2.25 | 0.88 |
| 82:4:6189:G:H2' | 82:4:6190:U:C6 | 2.08 | 0.88 |
| 1:5:2481:C:OP1 | 10:GG:244:LYS:HE3 | 1.73 | 0.88 |
| 17:OO:190[A]:VAL:O | 17:OO:192[A]:GLU:N | 2.06 | 0.88 |
| 83:1:583:HIS:CE1 | 83:1:704:GLN:HB3 | 2.08 | 0.88 |
| 17:OO:153[A]:VAL:CG1 | 17:OO:153[A]:VAL:O | 2.21 | 0.88 |
| 1:5:2239:A:H2' | 1:5:2240:A:H8 | 1.32 | 0.88 |
| 1:5:2481:C:H2' | 1:5:2482:U:C5 | 2.08 | 0.88 |
| 1:5:3237:U:O2' | 8:EE:127:LYS:HD2 | 1.74 | 0.88 |
| 17:OO:126[A]:ARG:HD3 | 17:OO:136[A]:TYR:CD2 | 2.09 | 0.88 |
| 17:OO:20[A]:LEU:O | 17:OO:20[A]:LEU:HG | 1.73 | 0.88 |
| 17:OO:138[A]:THR:O | 17:OO:139[A]:LEU:C | 2.11 | 0.87 |
| 83:1:694:HIS:CD2 | 83:1:700:ARG:NH2 | 2.42 | 0.87 |
| 82:4:6120:U:C1' | 82:4:6127:C:H5'' | 2.04 | 0.87 |
| 17:OO:86[A]:ARG:O | 17:OO:86[A]:ARG:CD | 2.20 | 0.87 |
| 17:OO:95[A]:ARG:O | 17:OO:95[A]:ARG:CG | 2.21 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|-----------------------|--------------------------|-------------------|
| 1:5:2234:C:O2' | 1:5:2235:U:O4' | 1.93 | 0.87 |
| 1:5:1925:G:H2' | 1:5:2055:G:N2 | 1.89 | 0.87 |
| 83:1:381:TYR:O | 83:1:382:VAL:HG23 | 1.74 | 0.87 |
| 81:2:1439:C:O2' | 81:2:1440:U:H5' | 1.75 | 0.87 |
| 1:5:1925:G:N3 | 1:5:2056:C:N1 | 2.09 | 0.87 |
| 17:OO:85[A]:VAL:O | 17:OO:88[A]:MET:N | 2.02 | 0.87 |
| 83:1:682:ARG:NH2 | 83:1:801:TRP:HE3 | 1.73 | 0.87 |
| 81:2:628:U:C4 | 81:2:969:A:N6 | 2.43 | 0.87 |
| 1:5:2167:A:H1' | 1:5:2238:U:O4' | 1.74 | 0.86 |
| 83:1:694:HIS:ND1 | 83:1:696:ASP:OD1 | 2.07 | 0.86 |
| 1:5:1925:G:N7 | 1:5:2057:A:N3 | 2.24 | 0.86 |
| 83:1:580:PRO:CD | 83:1:583:HIS:CD2 | 2.57 | 0.86 |
| 83:1:578:LYS:HE2 | 83:1:585:ARG:HH12 | 1.41 | 0.86 |
| 17:OO:120[A]:VAL:HG23 | 17:OO:120[A]:VAL:O | 1.76 | 0.86 |
| 83:1:564:ARG:HD2 | 83:1:681:MET:HG3 | 1.56 | 0.86 |
| 81:2:1292:U:O4 | 81:2:1321:A:C6 | 2.29 | 0.86 |
| 3:8:8:C:O2' | 3:8:9:A:H5' | 1.74 | 0.86 |
| 81:2:628:U:N3 | 81:2:969:A:C6 | 2.44 | 0.86 |
| 1:5:2218:G:C1' | 1:5:2219:G:H5' | 2.05 | 0.86 |
| 82:4:6181:C:C3' | 83:1:578:LYS:NZ | 2.38 | 0.85 |
| 82:4:6119:U:H5' | 82:4:6120:U:H5'' | 1.58 | 0.85 |
| 1:5:1923:G:H8 | 1:5:1923:G:O5' | 1.59 | 0.85 |
| 1:5:957:U:O2 | 1:5:958:U:C6 | 2.28 | 0.85 |
| 17:OO:19[A]:ARG:C | 17:OO:21[A]:ALA:H | 1.74 | 0.85 |
| 83:1:685:ARG:HG2 | 83:1:685:ARG:HH11 | 1.41 | 0.85 |
| 1:5:2229:U:OP2 | 81:2:1643:G:O2' | 1.91 | 0.85 |
| 17:OO:141[A]:LYS:O | 17:OO:143[A]:SER:N | 2.09 | 0.85 |
| 17:OO:23[A]:THR:O | 17:OO:25[A]:ALA:N | 2.09 | 0.85 |
| 83:1:586:ILE:HD11 | 83:1:708:THR:HG1 | 1.39 | 0.85 |
| 1:5:2055:G:C4 | 1:5:2056:C:N3 | 2.45 | 0.85 |
| 83:1:567:VAL:HG11 | 83:1:684:VAL:HG22 | 1.57 | 0.85 |
| 81:2:480:A:C2 | 81:2:506:U:O4 | 2.29 | 0.85 |
| 83:1:647:ILE:HB | 83:1:685:ARG:HH12 | 1.42 | 0.84 |
| 17:OO:93[A]:THR:O | 17:OO:95[A]:ARG:N | 2.09 | 0.84 |
| 17:OO:95[A]:ARG:O | 17:OO:95[A]:ARG:HG2 | 1.77 | 0.84 |
| 83:1:204:PRO:CG | 83:1:245:TRP:CZ2 | 2.60 | 0.84 |
| 1:5:1928:A:N1 | 1:5:2053:C:H2' | 1.91 | 0.84 |
| 17:OO:44[A]:ILE:CD1 | 17:OO:139[A]:LEU:HD11 | 2.07 | 0.84 |
| 81:2:928:A:C2' | 81:2:929:A:C5' | 2.56 | 0.84 |
| 83:1:381:TYR:O | 83:1:382:VAL:CB | 2.21 | 0.84 |
| 83:1:701:GLY:O | 83:1:705:ILE:HD12 | 1.77 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|-----------------------|--------------------------|-------------------|
| 83:1:806:SER:OG | 83:1:815:ALA:N | 2.10 | 0.84 |
| 1:5:2050:A:HO2' | 1:5:2051:U:P | 2.01 | 0.84 |
| 83:1:580:PRO:HD2 | 83:1:583:HIS:ND1 | 1.93 | 0.84 |
| 1:5:2218:G:C2 | 1:5:2219:G:C5 | 2.65 | 0.84 |
| 1:5:436:A:N1 | 1:5:596:U:O4 | 2.10 | 0.84 |
| 17:OO:34[A]:ILE:O | 17:OO:35[A]:VAL:HB | 1.76 | 0.84 |
| 17:OO:13[A]:LYS:HD2 | 17:OO:38[A]:ARG:HH22 | 1.41 | 0.84 |
| 83:1:638:PRO:CD | 83:1:681:MET:HE2 | 2.07 | 0.83 |
| 17:OO:75[A]:ARG:NE | 17:OO:146[A]:VAL:O | 2.10 | 0.83 |
| 3:8:9:A:H2' | 3:8:10:A:C8 | 2.13 | 0.83 |
| 17:OO:111[A]:PRO:CB | 17:OO:112[A]:PRO:CD | 2.54 | 0.83 |
| 17:OO:127[A]:VAL:HG13 | 17:OO:127[A]:VAL:O | 1.78 | 0.83 |
| 17:OO:55[A]:TYR:C | 17:OO:57[A]:ASP:H | 1.80 | 0.83 |
| 1:5:2479:U:O2' | 1:5:2480:A:H5' | 1.77 | 0.83 |
| 17:OO:111[A]:PRO:HB2 | 17:OO:112[A]:PRO:HD3 | 1.60 | 0.83 |
| 17:OO:176[A]:ASN:O | 17:OO:177[A]:ALA:C | 2.17 | 0.83 |
| 17:OO:20[A]:LEU:HD12 | 17:OO:20[A]:LEU:C | 1.92 | 0.83 |
| 1:5:1925:G:C2 | 1:5:2056:C:C2 | 2.59 | 0.83 |
| 1:5:1927:G:C6 | 1:5:2054:U:H2' | 2.12 | 0.83 |
| 1:5:1925:G:C4 | 1:5:2056:C:C2 | 2.65 | 0.83 |
| 81:2:22:A:O2' | 81:2:23:G:H5' | 1.78 | 0.83 |
| 83:1:463:LEU:HD11 | 83:1:467:GLY:CA | 2.09 | 0.82 |
| 83:1:694:HIS:HD2 | 83:1:700:ARG:HH22 | 1.23 | 0.82 |
| 17:OO:141[A]:LYS:O | 17:OO:144[A]:THR:N | 2.12 | 0.82 |
| 17:OO:86[A]:ARG:HB2 | 17:OO:100[A]:LEU:HD13 | 1.60 | 0.82 |
| 81:2:928:A:H2' | 81:2:929:A:C5' | 2.07 | 0.82 |
| 1:5:430:U:H2' | 1:5:431:U:C6 | 2.13 | 0.82 |
| 83:1:244:LEU:O | 83:1:245:TRP:HB2 | 1.80 | 0.82 |
| 83:1:586:ILE:HG22 | 83:1:587:TYR:H | 1.44 | 0.82 |
| 83:1:586:ILE:HG23 | 83:1:688:ILE:HD11 | 1.62 | 0.82 |
| 1:5:2480:A:O5' | 1:5:2481:C:H5'' | 1.80 | 0.82 |
| 17:OO:9[A]:VAL:HA | 17:OO:35[A]:VAL:HG12 | 1.58 | 0.82 |
| 17:OO:173[A]:LYS:O | 17:OO:174[A]:ALA:C | 2.18 | 0.82 |
| 17:OO:187[A]:GLY:O | 17:OO:189[A]:GLU:N | 2.12 | 0.82 |
| 83:1:381:TYR:O | 83:1:382:VAL:CG2 | 2.28 | 0.82 |
| 17:OO:44[A]:ILE:HD11 | 17:OO:139[A]:LEU:CD1 | 2.08 | 0.82 |
| 83:1:587:TYR:CG | 83:1:689:LEU:O | 2.33 | 0.82 |
| 83:1:695:ALA:C | 83:1:700:ARG:HH11 | 1.81 | 0.82 |
| 1:5:1190:C:O2' | 1:5:1257:A:N1 | 2.12 | 0.82 |
| 1:5:1925:G:N3 | 1:5:2056:C:H2' | 1.95 | 0.82 |
| 1:5:1928:A:C2 | 1:5:2053:C:C2' | 2.62 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:5:2480:A:H2' | 1:5:2481:C:C1' | 2.09 | 0.82 |
| 83:1:693:LEU:CB | 83:1:695:ALA:HA | 2.04 | 0.82 |
| 81:2:884:G:H2' | 81:2:885:U:N1 | 1.94 | 0.82 |
| 17:OO:27[A]:GLN:O | 17:OO:28[A]:LEU:HD23 | 1.79 | 0.81 |
| 17:OO:33[A]:LYS:O | 17:OO:34[A]:ILE:CG1 | 2.27 | 0.81 |
| 83:1:583:HIS:CE1 | 83:1:704:GLN:CD | 2.51 | 0.81 |
| 83:1:685:ARG:HB3 | 83:1:686:VAL:HA | 1.61 | 0.81 |
| 17:OO:34[A]:ILE:CG2 | 17:OO:35[A]:VAL:N | 2.09 | 0.81 |
| 83:1:584:ASN:ND2 | 83:1:693:LEU:CD1 | 2.42 | 0.81 |
| 17:OO:99[A]:ALA:O | 17:OO:101[A]:GLU:N | 2.13 | 0.81 |
| 1:5:1554:C:H2' | 1:5:1555:G:H5' | 1.62 | 0.81 |
| 1:5:2167:A:N7 | 1:5:2238:U:C4 | 2.49 | 0.81 |
| 15:MM:15:VAL:HG23 | 15:MM:35:ILE:HD13 | 1.60 | 0.81 |
| 14:LL:5:LYS:O | 14:LL:6:ASN:C | 2.18 | 0.81 |
| 14:LL:5:LYS:O | 14:LL:7:LEU:HB2 | 1.80 | 0.81 |
| 1:5:2235:U:H2' | 1:5:2236:C:C5 | 2.15 | 0.81 |
| 17:OO:91[A]:HIS:O | 17:OO:91[A]:HIS:CG | 2.29 | 0.81 |
| 14:LL:5:LYS:O | 14:LL:7:LEU:N | 2.14 | 0.81 |
| 1:5:2218:G:C2 | 1:5:2219:G:C4 | 2.69 | 0.81 |
| 17:OO:58[A]:TYR:O | 17:OO:60[A]:ARG:N | 2.13 | 0.81 |
| 83:1:578:LYS:HE2 | 83:1:585:ARG:NH1 | 1.95 | 0.81 |
| 83:1:694:HIS:H | 83:1:700:ARG:HH12 | 0.86 | 0.81 |
| 1:5:2217:C:O2' | 1:5:2218:G:OP1 | 1.99 | 0.81 |
| 1:5:529:U:C4 | 1:5:532:A:N6 | 2.49 | 0.81 |
| 1:5:2285:G:O2' | 1:5:2286:A:H5' | 1.80 | 0.80 |
| 17:OO:156[A]:LYS:O | 17:OO:158[A]:GLU:N | 2.14 | 0.80 |
| 83:1:587:TYR:HE2 | 83:1:691:VAL:H | 0.95 | 0.80 |
| 82:4:6120:U:H1' | 82:4:6127:C:C5' | 2.10 | 0.80 |
| 3:8:8:C:O2' | 3:8:9:A:C5' | 2.28 | 0.80 |
| 17:OO:68[A]:THR:O | 17:OO:72[A]:PHE:CE1 | 2.34 | 0.80 |
| 81:2:480:A:C6 | 81:2:506:U:O4 | 2.34 | 0.80 |
| 1:5:2285:G:O2' | 1:5:2286:A:C5' | 2.29 | 0.80 |
| 17:OO:148[A]:TRP:CH2 | 17:OO:150[A]:TYR:O | 2.34 | 0.80 |
| 83:1:383:SER:O | 83:1:465:LYS:O | 1.99 | 0.80 |
| 83:1:695:ALA:CA | 83:1:700:ARG:NH1 | 2.44 | 0.80 |
| 81:2:886:A:C2 | 81:2:925:A:H2 | 1.96 | 0.80 |
| 1:5:2167:A:C5 | 1:5:2238:U:O4 | 2.23 | 0.80 |
| 1:5:1923:G:C2 | 1:5:1925:G:C8 | 2.68 | 0.80 |
| 1:5:2480:A:H2' | 1:5:2481:C:O4' | 1.82 | 0.80 |
| 17:OO:9[A]:VAL:HG22 | 17:OO:35[A]:VAL:CG1 | 2.11 | 0.80 |
| 1:5:2479:U:C2 | 1:5:2480:A:C8 | 2.70 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 17:OO:9[A]:VAL:HG12 | 17:OO:118[A]:ARG:HB3 | 1.63 | 0.80 |
| 1:5:2481:C:OP1 | 10:GG:245:ILE:HG13 | 1.83 | 0.79 |
| 82:4:6121:A:C6 | 82:4:6158:A:C2 | 2.70 | 0.79 |
| 1:5:2234:C:C2' | 1:5:2235:U:O4' | 2.31 | 0.79 |
| 6:CC:349:ILE:CG1 | 6:CC:350:LYS:HG3 | 2.11 | 0.79 |
| 12:II:14:ASN:O | 12:II:128:ARG:NH2 | 2.16 | 0.79 |
| 1:5:2238:U:C5 | 1:5:2239:A:N7 | 2.51 | 0.79 |
| 83:1:381:TYR:O | 83:1:382:VAL:HB | 1.81 | 0.79 |
| 17:OO:173[A]:LYS:O | 17:OO:176[A]:ASN:N | 2.15 | 0.79 |
| 17:OO:86[A]:ARG:CB | 17:OO:100[A]:LEU:CD1 | 2.45 | 0.79 |
| 1:5:2237:U:OP1 | 82:4:6205:DA:OP1 | 2.00 | 0.79 |
| 17:OO:97[A]:LYS:O | 17:OO:101[A]:GLU:HG3 | 1.83 | 0.79 |
| 17:OO:5[A]:GLU:CA | 17:OO:5[A]:GLU:OE1 | 2.31 | 0.79 |
| 83:1:806:SER:CB | 83:1:813:SER:HB2 | 2.12 | 0.79 |
| 17:OO:158[A]:GLU:O | 17:OO:159[A]:GLU:C | 2.19 | 0.78 |
| 83:1:380:LEU:HB3 | 83:1:400:VAL:HA | 1.65 | 0.78 |
| 81:2:886:A:C2 | 81:2:925:A:N1 | 2.51 | 0.78 |
| 17:OO:86[A]:ARG:CA | 17:OO:100[A]:LEU:HD11 | 2.13 | 0.78 |
| 17:OO:120[A]:VAL:CG2 | 17:OO:120[A]:VAL:O | 2.32 | 0.78 |
| 83:1:586:ILE:HA | 83:1:691:VAL:HG22 | 1.65 | 0.78 |
| 81:2:1292:U:C4 | 81:2:1321:A:C2 | 2.71 | 0.78 |
| 3:8:26:U:H2' | 3:8:27:U:C6 | 2.18 | 0.78 |
| 83:1:587:TYR:CG | 83:1:689:LEU:C | 2.57 | 0.78 |
| 1:5:2055:G:C4 | 1:5:2056:C:C4 | 2.72 | 0.78 |
| 1:5:2217:C:C4' | 1:5:2218:G:H5' | 2.11 | 0.78 |
| 1:5:2238:U:C4 | 1:5:2239:A:C4 | 2.72 | 0.78 |
| 1:5:2482:U:C5 | 1:5:2560:G:C6 | 2.71 | 0.78 |
| 82:4:6039:A:N6 | 82:4:6087:G:OP1 | 2.17 | 0.78 |
| 83:1:567:VAL:CG1 | 83:1:684:VAL:HG22 | 2.13 | 0.78 |
| 82:4:6119:U:H5' | 82:4:6120:U:H5' | 1.64 | 0.78 |
| 1:5:2239:A:C2' | 1:5:2240:A:C8 | 2.65 | 0.78 |
| 6:CC:349:ILE:HG23 | 6:CC:350:LYS:HE3 | 1.66 | 0.78 |
| 17:OO:148[A]:TRP:CZ2 | 17:OO:150[A]:TYR:O | 2.36 | 0.78 |
| 1:5:504:A:N6 | 1:5:529:U:C5 | 2.52 | 0.78 |
| 17:OO:194[A]:LEU:C | 17:OO:196[A]:ALA:N | 2.36 | 0.78 |
| 83:1:806:SER:OG | 83:1:815:ALA:CA | 2.31 | 0.78 |
| 1:5:2167:A:N1 | 1:5:2238:U:C5 | 2.52 | 0.78 |
| 17:OO:43[A]:ASN:OD1 | 17:OO:136[A]:TYR:CE2 | 2.37 | 0.78 |
| 17:OO:169[A]:TYR:O | 17:OO:169[A]:TYR:CD1 | 2.37 | 0.78 |
| 17:OO:27[A]:GLN:O | 17:OO:32[A]:GLN:HB3 | 1.84 | 0.78 |
| 1:5:2234:C:H2' | 1:5:2235:U:O4' | 1.83 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 1:5:2481:C:O5' | 10:GG:244:LYS:CE | 2.24 | 0.78 |
| 17:OO:161[A]:ARG:HG2 | 17:OO:162[A]:LYS:H | 1.48 | 0.78 |
| 17:OO:65[A]:PHE:CG | 17:OO:65[A]:PHE:O | 2.35 | 0.78 |
| 83:1:682:ARG:NH2 | 83:1:801:TRP:CE3 | 2.49 | 0.77 |
| 83:1:576:LEU:HD22 | 83:1:587:TYR:CD1 | 2.16 | 0.77 |
| 8:EE:13:VAL:CG2 | 8:EE:14:PRO:CD | 2.29 | 0.77 |
| 1:5:647:G:O6 | 19:QQ:56:LYS:NZ | 2.17 | 0.77 |
| 17:OO:107[A]:GLU:OE2 | 17:OO:107[A]:GLU:C | 2.23 | 0.77 |
| 17:OO:16[A]:LEU:HA | 17:OO:43[A]:ASN:O | 1.83 | 0.77 |
| 17:OO:194[A]:LEU:C | 17:OO:196[A]:ALA:H | 1.86 | 0.77 |
| 83:1:379:MET:SD | 83:1:380:LEU:CD2 | 2.71 | 0.77 |
| 1:5:1924:C:H4' | 1:5:1925:G:OP1 | 1.85 | 0.77 |
| 1:5:2055:G:C5 | 1:5:2056:C:C4 | 2.72 | 0.77 |
| 4:AA:196:TRP:CE3 | 4:AA:197:PRO:HD3 | 2.19 | 0.77 |
| 83:1:380:LEU:HD13 | 83:1:400:VAL:CB | 2.14 | 0.77 |
| 1:5:1924:C:O2' | 1:5:1925:G:H3' | 1.84 | 0.77 |
| 17:OO:82[A]:TYR:C | 17:OO:82[A]:TYR:CD1 | 2.57 | 0.77 |
| 81:2:1590:A:H2' | 81:2:1591:A:C8 | 2.19 | 0.77 |
| 82:4:6039:A:N3 | 82:4:6039:A:H2' | 1.99 | 0.77 |
| 17:OO:145[A]:SER:O | 17:OO:146[A]:VAL:HG12 | 1.82 | 0.77 |
| 17:OO:76[A]:ALA:O | 17:OO:78[A]:SER:N | 2.18 | 0.77 |
| 1:5:2238:U:C4 | 1:5:2239:A:C5 | 2.72 | 0.77 |
| 1:5:78:U:H3 | 1:5:325:A:N6 | 1.83 | 0.77 |
| 17:OO:23[A]:THR:C | 17:OO:25[A]:ALA:H | 1.88 | 0.77 |
| 17:OO:192[A]:GLU:O | 17:OO:193[A]:LYS:C | 2.22 | 0.77 |
| 54:G:154:ARG:HA | 81:2:78:A:H3' | 1.66 | 0.77 |
| 17:OO:104[A]:LYS:O | 17:OO:105[A]:VAL:HG22 | 1.85 | 0.77 |
| 17:OO:65[A]:PHE:O | 17:OO:66[A]:ASN:CB | 2.33 | 0.77 |
| 17:OO:171[A]:LYS:NZ | 17:OO:171[A]:LYS:HB3 | 2.00 | 0.76 |
| 17:OO:66[A]:ASN:O | 17:OO:68[A]:THR:N | 2.17 | 0.76 |
| 1:5:1924:C:C4 | 1:5:2055:G:O6 | 2.37 | 0.76 |
| 4:AA:3:ARG:NH1 | 4:AA:208:ASP:OD1 | 2.18 | 0.76 |
| 17:OO:94[A]:ALA:C | 17:OO:96[A]:GLY:H | 1.88 | 0.76 |
| 81:2:884:G:O2' | 81:2:885:U:C1' | 2.27 | 0.76 |
| 17:OO:32[A]:GLN:O | 17:OO:102[A]:ARG:HD3 | 1.86 | 0.76 |
| 81:2:749:U:H2' | 81:2:750:U:C6 | 2.19 | 0.76 |
| 82:4:6120:U:O2' | 82:4:6127:C:H5'' | 1.85 | 0.76 |
| 5:BB:229:VAL:HG11 | 5:BB:249:VAL:HG23 | 1.68 | 0.76 |
| 6:CC:350:LYS:HD2 | 6:CC:350:LYS:N | 2.00 | 0.76 |
| 9:FF:105:LEU:HD21 | 9:FF:112:THR:HG23 | 1.67 | 0.76 |
| 17:OO:97[A]:LYS:O | 17:OO:98[A]:ALA:C | 2.22 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|-----------------------|--------------------------|-------------------|
| 83:1:579:SER:OG | 83:1:580:PRO:HD3 | 1.86 | 0.76 |
| 17:OO:137[A]:THR:HG22 | 17:OO:138[A]:THR:N | 1.97 | 0.76 |
| 82:4:6181:C:H3' | 83:1:578:LYS:CE | 2.16 | 0.76 |
| 83:1:586:ILE:HD11 | 83:1:708:THR:CB | 2.16 | 0.76 |
| 17:OO:122[A]:PRO:HA | 17:OO:125[A]:LEU:HD23 | 1.67 | 0.76 |
| 83:1:380:LEU:HD12 | 83:1:400:VAL:CA | 2.11 | 0.75 |
| 83:1:695:ALA:HA | 83:1:700:ARG:NH1 | 2.01 | 0.75 |
| 83:1:705:ILE:HA | 83:1:708:THR:HG21 | 1.64 | 0.75 |
| 57:J:14:THR:CG2 | 81:2:23:G:P | 2.68 | 0.75 |
| 83:1:586:ILE:CG2 | 83:1:688:ILE:HD11 | 2.16 | 0.75 |
| 1:5:436:A:N1 | 1:5:596:U:C4 | 2.53 | 0.75 |
| 1:5:2218:G:C2 | 1:5:2219:G:N9 | 2.55 | 0.75 |
| 17:OO:17[A]:LEU:O | 17:OO:19[A]:ARG:N | 2.19 | 0.75 |
| 17:OO:34[A]:ILE:HG23 | 17:OO:35[A]:VAL:H | 1.46 | 0.75 |
| 17:OO:76[A]:ALA:O | 17:OO:77[A]:PRO:C | 2.25 | 0.75 |
| 81:2:8:U:O4 | 81:2:1138:A:N6 | 2.18 | 0.75 |
| 1:5:1083:A:OP2 | 14:LL:5:LYS:NZ | 2.18 | 0.75 |
| 81:2:928:A:O2' | 81:2:929:A:H5'' | 1.85 | 0.75 |
| 1:5:958:U:H2' | 1:5:959:U:C6 | 2.22 | 0.75 |
| 17:OO:143[A]:SER:O | 17:OO:145[A]:SER:N | 2.19 | 0.75 |
| 1:5:529:U:C2 | 1:5:532:A:N6 | 2.54 | 0.74 |
| 1:5:2393:A:H2' | 1:5:2394:G:O4' | 1.86 | 0.74 |
| 1:5:1197:G:C5 | 1:5:1198:C:C4 | 2.74 | 0.74 |
| 1:5:298:U:H4' | 1:5:299:G:H5' | 1.70 | 0.74 |
| 17:OO:23[A]:THR:C | 17:OO:25[A]:ALA:N | 2.39 | 0.74 |
| 1:5:2260:A:O2' | 81:2:1653:A:N1 | 2.19 | 0.74 |
| 81:2:885:U:H2' | 81:2:886:A:H5'' | 1.67 | 0.74 |
| 82:4:6181:C:H3' | 83:1:578:LYS:HZ3 | 1.45 | 0.74 |
| 83:1:517:CYS:SG | 83:1:518:VAL:N | 2.61 | 0.74 |
| 81:2:945:U:H2' | 81:2:946:U:C6 | 2.23 | 0.74 |
| 17:OO:31[A]:GLY:O | 17:OO:32[A]:GLN:C | 2.24 | 0.74 |
| 17:OO:43[A]:ASN:OD1 | 17:OO:136[A]:TYR:HE2 | 1.71 | 0.74 |
| 1:5:2167:A:C4 | 1:5:2238:U:C4 | 2.52 | 0.74 |
| 17:OO:114[A]:ASP:HA | 17:OO:118[A]:ARG:NH1 | 1.99 | 0.74 |
| 83:1:695:ALA:O | 83:1:700:ARG:CZ | 2.36 | 0.74 |
| 81:2:11:A:O2' | 81:2:12:U:O5' | 2.01 | 0.74 |
| 1:5:1923:G:C6 | 1:5:2057:A:H2 | 2.05 | 0.74 |
| 1:5:2481:C:P | 10:GG:244:LYS:HE2 | 2.21 | 0.74 |
| 81:2:886:A:N7 | 81:2:887:U:C5 | 2.56 | 0.74 |
| 83:1:380:LEU:CD1 | 83:1:400:VAL:N | 2.51 | 0.74 |
| 1:5:2218:G:H1' | 1:5:2219:G:C5' | 2.11 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 11:HH:41:ILE:HD12 | 11:HH:43:VAL:HG13 | 1.69 | 0.74 |
| 17:OO:9[A]:VAL:HA | 17:OO:35[A]:VAL:CG1 | 2.17 | 0.74 |
| 83:1:580:PRO:CG | 83:1:583:HIS:CE1 | 2.70 | 0.73 |
| 1:5:2055:G:C2 | 1:5:2056:C:N3 | 2.56 | 0.73 |
| 1:5:520:G:H2' | 1:5:521:U:H5' | 1.70 | 0.73 |
| 17:OO:103[A]:LEU:O | 17:OO:103[A]:LEU:HG | 1.87 | 0.73 |
| 1:5:2218:G:C2 | 1:5:2219:G:N7 | 2.56 | 0.73 |
| 1:5:2284:G:O2' | 1:5:2285:G:H5' | 1.88 | 0.73 |
| 6:CC:349:ILE:HG13 | 6:CC:350:LYS:CA | 2.18 | 0.73 |
| 54:G:155:ASP:HB2 | 81:2:77:U:O3' | 1.87 | 0.73 |
| 17:OO:107[A]:GLU:CA | 17:OO:107[A]:GLU:OE2 | 2.35 | 0.73 |
| 83:1:30:HIS:CE1 | 83:1:133:GLU:OE1 | 2.41 | 0.73 |
| 83:1:647:ILE:HB | 83:1:685:ARG:NH1 | 2.02 | 0.73 |
| 49:B:117:TRP:H | 81:2:931:U:P | 2.11 | 0.73 |
| 1:5:78:U:H3 | 1:5:325:A:H61 | 1.36 | 0.73 |
| 82:4:6181:C:C2' | 83:1:578:LYS:NZ | 2.43 | 0.73 |
| 83:1:702:GLY:HA3 | 83:1:706:ILE:HD12 | 1.67 | 0.73 |
| 81:2:1439:C:H2' | 81:2:1440:U:H5' | 1.69 | 0.73 |
| 1:5:1194:A:H1' | 1:5:1195:C:O4' | 1.88 | 0.73 |
| 14:LL:3:ILE:HG13 | 14:LL:4:SER:H | 1.53 | 0.73 |
| 1:5:2167:A:O4' | 1:5:2238:U:H1' | 1.88 | 0.73 |
| 17:OO:145[A]:SER:O | 17:OO:146[A]:VAL:HG13 | 1.87 | 0.73 |
| 17:OO:161[A]:ARG:O | 17:OO:162[A]:LYS:C | 2.25 | 0.73 |
| 1:5:529:U:O2 | 1:5:532:A:N7 | 2.22 | 0.73 |
| 83:1:157:ILE:CD1 | 83:1:211:PHE:CE1 | 2.71 | 0.73 |
| 1:5:2505:A:O3' | 49:B:226:GLY:O | 2.07 | 0.73 |
| 17:OO:145[A]:SER:C | 17:OO:146[A]:VAL:HG13 | 2.08 | 0.73 |
| 83:1:589:LYS:CD | 83:1:685:ARG:HD2 | 2.18 | 0.72 |
| 1:5:1033:A:C2 | 1:5:1069:A:C6 | 2.77 | 0.72 |
| 1:5:1927:G:O6 | 1:5:2054:U:H2' | 1.88 | 0.72 |
| 1:5:2479:U:H2' | 1:5:2480:A:O4' | 1.89 | 0.72 |
| 1:5:529:U:O2 | 1:5:532:A:C5 | 2.42 | 0.72 |
| 17:OO:47[A]:GLU:HG3 | 17:OO:47[A]:GLU:O | 1.89 | 0.72 |
| 17:OO:7[A]:VAL:HG12 | 17:OO:8[A]:VAL:N | 2.03 | 0.72 |
| 83:1:698:ILE:CB | 83:1:699:HIS:C | 2.48 | 0.72 |
| 70:W:40:VAL:HG11 | 70:W:103:ILE:HD12 | 1.71 | 0.72 |
| 17:OO:168[A]:TYR:C | 17:OO:168[A]:TYR:CD1 | 2.61 | 0.72 |
| 83:1:580:PRO:HG2 | 83:1:583:HIS:CE1 | 2.22 | 0.72 |
| 1:5:2238:U:C5 | 1:5:2239:A:C8 | 2.78 | 0.72 |
| 1:5:943:A:H2' | 1:5:944:A:O4' | 1.88 | 0.72 |
| 17:OO:161[A]:ARG:HG2 | 17:OO:162[A]:LYS:N | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 17:OO:38[A]:ARG:O | 17:OO:39[A]:ALA:C | 2.28 | 0.72 |
| 81:2:10:G:H8 | 81:2:1631:A:HO2' | 1.35 | 0.72 |
| 1:5:1925:G:N1 | 1:5:2056:C:C4 | 2.58 | 0.72 |
| 1:5:2480:A:H3' | 1:5:2481:C:C4' | 2.20 | 0.72 |
| 17:OO:27[A]:GLN:C | 17:OO:28[A]:LEU:HD23 | 2.09 | 0.72 |
| 83:1:702:GLY:HA2 | 83:1:706:ILE:HG13 | 1.71 | 0.72 |
| 1:5:1924:C:N4 | 1:5:2055:G:C6 | 2.57 | 0.72 |
| 17:OO:193[A]:LYS:HE3 | 17:OO:193[A]:LYS:CA | 2.17 | 0.72 |
| 57:J:14:THR:HG21 | 81:2:22:A:O3' | 1.89 | 0.71 |
| 81:2:884:G:O3' | 81:2:885:U:H4' | 1.90 | 0.71 |
| 1:5:2237:U:N3 | 1:5:2241:G:C6 | 2.54 | 0.71 |
| 1:5:2167:A:C8 | 1:5:2238:U:C2 | 2.77 | 0.71 |
| 1:5:2480:A:H2' | 1:5:2481:C:C4' | 2.21 | 0.71 |
| 48:A:73:VAL:HG13 | 48:A:120:LEU:HD12 | 1.72 | 0.71 |
| 1:5:1693:U:H1' | 1:5:1694:C:C6 | 2.25 | 0.71 |
| 1:5:2238:U:H2' | 1:5:2239:A:O4' | 1.90 | 0.71 |
| 3:8:145:U:H2' | 3:8:146:U:C6 | 2.25 | 0.71 |
| 17:OO:31[A]:GLY:C | 17:OO:32[A]:GLN:O | 2.26 | 0.71 |
| 81:2:1173:C:N3 | 81:2:1464:G:C2 | 2.58 | 0.71 |
| 10:GG:74:ILE:O | 10:GG:76:GLN:N | 2.24 | 0.71 |
| 1:5:1867:G:O2' | 24:VV:21:ALA:HB2 | 1.90 | 0.71 |
| 83:1:681:MET:HB3 | 83:1:682:ARG:HG3 | 1.73 | 0.71 |
| 1:5:52:A:N3 | 1:5:782:U:O2' | 2.23 | 0.71 |
| 54:G:154:ARG:CA | 81:2:78:A:O5' | 2.39 | 0.71 |
| 5:BB:56:ILE:HD12 | 5:BB:76:VAL:HG21 | 1.72 | 0.71 |
| 17:OO:97[A]:LYS:O | 17:OO:98[A]:ALA:O | 2.08 | 0.71 |
| 5:BB:283:TYR:HB2 | 5:BB:323:ILE:HG22 | 1.73 | 0.70 |
| 83:1:371:ASN:O | 83:1:372:CYS:HB3 | 1.91 | 0.70 |
| 83:1:577:SER:HB2 | 83:1:585:ARG:HA | 1.72 | 0.70 |
| 83:1:587:TYR:HE2 | 83:1:690:ASP:CA | 1.83 | 0.70 |
| 1:5:1927:G:O6 | 1:5:2055:G:C8 | 2.44 | 0.70 |
| 5:BB:382:THR:N | 5:BB:383:LEU:HB3 | 2.07 | 0.70 |
| 17:OO:7[A]:VAL:HG13 | 17:OO:8[A]:VAL:N | 2.04 | 0.70 |
| 1:5:2480:A:H2' | 1:5:2481:C:H1' | 1.71 | 0.70 |
| 48:A:120:LEU:HD11 | 48:A:144:ILE:HD12 | 1.73 | 0.70 |
| 17:OO:129[A]:ARG:O | 17:OO:131[A]:LYS:N | 2.25 | 0.70 |
| 1:5:2662:A:H2' | 1:5:2663:A:C8 | 2.25 | 0.70 |
| 6:CC:349:ILE:HG23 | 6:CC:350:LYS:HG3 | 1.73 | 0.70 |
| 81:2:1653:A:N6 | 81:2:1743:G:O2' | 2.25 | 0.70 |
| 1:5:2055:G:N3 | 1:5:2056:C:N3 | 2.40 | 0.70 |
| 1:5:2234:C:HO2' | 1:5:2235:U:C4' | 1.98 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:8:8:C:HO2' | 3:8:9:A:C5' | 2.03 | 0.70 |
| 14:LL:5:LYS:H | 14:LL:5:LYS:CD | 1.96 | 0.70 |
| 17:OO:82[A]:TYR:O | 17:OO:82[A]:TYR:CG | 2.43 | 0.70 |
| 83:1:806:SER:HB2 | 83:1:813:SER:CB | 2.19 | 0.69 |
| 27:YY:56:VAL:HG21 | 27:YY:104:VAL:HG13 | 1.72 | 0.69 |
| 83:1:647:ILE:CB | 83:1:685:ARG:HH12 | 2.05 | 0.69 |
| 81:2:884:G:H3' | 81:2:885:U:O4' | 1.88 | 0.69 |
| 1:5:2237:U:C4 | 1:5:2241:G:N1 | 2.49 | 0.69 |
| 83:1:244:LEU:O | 83:1:245:TRP:CB | 2.41 | 0.69 |
| 83:1:698:ILE:CA | 83:1:699:HIS:HB3 | 2.23 | 0.69 |
| 83:1:727:PRO:HB2 | 83:1:728:VAL:HA | 1.73 | 0.69 |
| 1:5:2055:G:N7 | 1:5:2056:C:N4 | 2.40 | 0.69 |
| 1:5:78:U:C4 | 1:5:325:A:N1 | 2.60 | 0.69 |
| 1:5:613:U:OP1 | 4:AA:21:ARG:NH2 | 79.44 | 0.69 |
| 63:P:18:LYS:O | 66:S:95:GLY:N | 2.24 | 0.69 |
| 6:CC:93:MET:N | 6:CC:93:MET:SD | 2.64 | 0.69 |
| 1:5:2218:G:C5 | 1:5:2219:G:C1' | 2.76 | 0.69 |
| 1:5:2238:U:O2' | 1:5:2239:A:H5' | 1.92 | 0.69 |
| 1:5:3023:U:H3 | 1:5:3055:A:H61 | 1.41 | 0.69 |
| 83:1:647:ILE:HG13 | 83:1:685:ARG:O | 1.93 | 0.69 |
| 81:2:406:A:O2' | 81:2:1669:A:N3 | 2.25 | 0.69 |
| 1:5:1574:A:O2' | 1:5:1576:U:OP2 | 2.08 | 0.69 |
| 1:5:1923:G:C8 | 1:5:1923:G:O5' | 2.44 | 0.69 |
| 1:5:2502:G:O2' | 1:5:2516:A:N1 | 2.22 | 0.69 |
| 1:5:520:G:H2' | 1:5:521:U:C5' | 2.22 | 0.69 |
| 49:B:114:VAL:HG21 | 81:2:929:A:C2 | 2.27 | 0.69 |
| 81:2:1085:A:H2' | 81:2:1086:A:C8 | 2.28 | 0.69 |
| 81:2:888:U:H2' | 81:2:889:C:C6 | 2.28 | 0.69 |
| 83:1:413:ILE:CG2 | 83:1:463:LEU:HD21 | 2.23 | 0.69 |
| 83:1:700:ARG:HG2 | 83:1:705:ILE:HD11 | 1.74 | 0.69 |
| 81:2:969:A:N6 | 81:2:970:A:C4 | 2.61 | 0.69 |
| 1:5:1579:G:H2' | 1:5:1580:G:O4' | 1.93 | 0.69 |
| 1:5:2481:C:O2' | 1:5:2482:U:C6 | 2.46 | 0.68 |
| 1:5:3077:G:C2 | 1:5:3094:C:C2 | 2.81 | 0.68 |
| 1:5:3077:G:N2 | 1:5:3094:C:C2 | 2.61 | 0.68 |
| 17:OO:169[A]:TYR:O | 17:OO:169[A]:TYR:CG | 2.45 | 0.68 |
| 83:1:380:LEU:HD12 | 83:1:400:VAL:HA | 1.74 | 0.68 |
| 83:1:703:GLY:H | 83:1:706:ILE:HB | 1.58 | 0.68 |
| 81:2:23:G:O2' | 81:2:24:U:O5' | 2.09 | 0.68 |
| 17:OO:57[A]:ASP:O | 17:OO:61[A]:LYS:NZ | 2.20 | 0.68 |
| 83:1:381:TYR:C | 83:1:382:VAL:HG23 | 2.12 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 83:1:583:HIS:ND1 | 83:1:704:GLN:HB3 | 2.08 | 0.68 |
| 81:2:1601:U:H2' | 81:2:1602:U:C6 | 2.28 | 0.68 |
| 62:O:81:ILE:HB | 62:O:115:ILE:HG22 | 1.75 | 0.68 |
| 17:OO:154[A]:VAL:O | 17:OO:154[A]:VAL:HG12 | 1.92 | 0.68 |
| 81:2:628:U:C2 | 81:2:969:A:N6 | 2.61 | 0.68 |
| 1:5:1925:G:C6 | 1:5:2056:C:C4 | 2.80 | 0.68 |
| 1:5:2239:A:C6 | 1:5:2240:A:C6 | 2.81 | 0.68 |
| 1:5:3023:U:H1' | 1:5:3025:U:OP2 | 1.93 | 0.68 |
| 17:OO:182[A]:LYS:O | 17:OO:184[A]:ALA:N | 2.26 | 0.68 |
| 1:5:78:U:H2' | 1:5:78:U:O2 | 1.93 | 0.68 |
| 17:OO:35[A]:VAL:HG21 | 17:OO:113[A]:TYR:CZ | 2.29 | 0.68 |
| 17:OO:176[A]:ASN:C | 17:OO:178[A]:VAL:N | 2.44 | 0.68 |
| 1:5:2438:G:C6 | 1:5:2439:C:N4 | 2.62 | 0.68 |
| 17:OO:99[A]:ALA:O | 17:OO:102[A]:ARG:N | 2.22 | 0.68 |
| 83:1:698:ILE:HB | 83:1:699:HIS:CA | 2.22 | 0.68 |
| 1:5:2237:U:O4 | 1:5:2241:G:C2 | 2.46 | 0.68 |
| 83:1:583:HIS:HE1 | 83:1:704:GLN:CG | 2.06 | 0.68 |
| 17:OO:126[A]:ARG:CD | 17:OO:136[A]:TYR:CD2 | 2.76 | 0.68 |
| 1:5:2167:A:O4' | 1:5:2238:U:C1' | 2.42 | 0.68 |
| 1:5:2281:A:O2' | 1:5:2284:G:N3 | 2.27 | 0.68 |
| 6:CC:104:LYS:O | 6:CC:106:TRP:N | 2.27 | 0.68 |
| 81:2:299:A:H2' | 81:2:300:A:C8 | 2.28 | 0.68 |
| 1:5:2218:G:N1 | 1:5:2219:G:C5 | 2.62 | 0.68 |
| 17:OO:159[A]:GLU:O | 17:OO:160[A]:LYS:C | 2.30 | 0.68 |
| 83:1:576:LEU:HD23 | 83:1:587:TYR:HA | 1.76 | 0.67 |
| 83:1:577:SER:OG | 83:1:586:ILE:HB | 1.94 | 0.67 |
| 81:2:1363:G:N2 | 81:2:1364:C:C2 | 2.62 | 0.67 |
| 1:5:336:A:C2 | 1:5:337:G:C5 | 2.81 | 0.67 |
| 17:OO:19[A]:ARG:C | 17:OO:21[A]:ALA:N | 2.38 | 0.67 |
| 17:OO:66[A]:ASN:C | 17:OO:68[A]:THR:H | 1.96 | 0.67 |
| 81:2:22:A:HO2' | 81:2:23:G:H5' | 1.59 | 0.67 |
| 1:5:2035:G:H2' | 1:5:2036:U:O4' | 1.94 | 0.67 |
| 83:1:381:TYR:O | 83:1:467:GLY:O | 2.12 | 0.67 |
| 17:OO:148[A]:TRP:CE2 | 17:OO:150[A]:TYR:O | 2.47 | 0.67 |
| 17:OO:63[A]:THR:HG22 | 17:OO:63[A]:THR:O | 1.94 | 0.67 |
| 57:J:170:GLY:C | 81:2:511:A:O4' | 2.32 | 0.67 |
| 81:2:886:A:C8 | 81:2:887:U:C5 | 2.82 | 0.67 |
| 82:4:6127:C:N3 | 82:4:6160:G:O6 | 2.27 | 0.67 |
| 83:1:702:GLY:C | 83:1:706:ILE:HD12 | 2.15 | 0.67 |
| 17:OO:32[A]:GLN:HG3 | 17:OO:33[A]:LYS:O | 1.95 | 0.67 |
| 81:2:884:G:O3' | 81:2:885:U:C4' | 2.42 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 1:5:2480:A:C6 | 1:5:2481:C:N3 | 2.63 | 0.67 |
| 17:OO:29[A]:LEU:HD23 | 17:OO:29[A]:LEU:N | 2.08 | 0.67 |
| 1:5:1044:U:H2' | 1:5:1045:U:C6 | 2.30 | 0.67 |
| 17:OO:148[A]:TRP:CZ3 | 17:OO:150[A]:TYR:O | 2.47 | 0.67 |
| 83:1:693:LEU:HB3 | 83:1:695:ALA:CA | 2.05 | 0.67 |
| 81:2:1046:G:C2 | 81:2:1071:C:C2 | 2.82 | 0.67 |
| 57:J:170:GLY:N | 81:2:511:A:OP1 | 2.23 | 0.67 |
| 1:5:1923:G:N1 | 1:5:2057:A:C2 | 2.62 | 0.67 |
| 83:1:581:ASN:N | 83:1:583:HIS:CD2 | 2.34 | 0.67 |
| 82:4:6120:U:C6 | 82:4:6127:C:H5' | 2.29 | 0.67 |
| 1:5:2217:C:C3' | 1:5:2218:G:C5' | 2.00 | 0.67 |
| 81:2:1793:U:O3' | 81:2:1795:A:N1 | 2.28 | 0.67 |
| 1:5:1147:C:H2' | 1:5:1148:G:N2 | 2.09 | 0.67 |
| 1:5:529:U:C2 | 1:5:532:A:C6 | 2.82 | 0.67 |
| 17:OO:172[A]:LYS:O | 17:OO:173[A]:LYS:C | 2.33 | 0.67 |
| 83:1:519:LEU:C | 83:1:519:LEU:HD12 | 2.15 | 0.66 |
| 54:G:154:ARG:CA | 81:2:78:A:H3' | 2.25 | 0.66 |
| 1:5:1925:G:C6 | 1:5:2057:A:C4 | 2.83 | 0.66 |
| 83:1:733:ILE:HG22 | 83:1:792:ALA:HB1 | 1.77 | 0.66 |
| 81:2:480:A:C2 | 81:2:506:U:C4 | 2.83 | 0.66 |
| 1:5:2237:U:P | 82:4:6205:DA:OP1 | 2.52 | 0.66 |
| 83:1:698:ILE:HG21 | 83:1:699:HIS:HD2 | 1.53 | 0.66 |
| 81:2:363:G:N2 | 81:2:380:C:C2 | 2.63 | 0.66 |
| 81:2:51:A:N6 | 81:2:439:U:H3 | 1.93 | 0.66 |
| 1:5:2167:A:C1' | 1:5:2238:U:O4' | 2.43 | 0.66 |
| 1:5:2482:U:O2' | 1:5:2483:U:C6 | 2.46 | 0.66 |
| 83:1:806:SER:CB | 83:1:815:ALA:H | 2.08 | 0.66 |
| 17:OO:9[A]:VAL:CG2 | 17:OO:35[A]:VAL:HG11 | 2.24 | 0.66 |
| 17:OO:42[A]:LEU:N | 17:OO:42[A]:LEU:HD13 | 2.09 | 0.66 |
| 81:2:928:A:O2' | 81:2:929:A:C5' | 2.44 | 0.66 |
| 17:OO:42[A]:LEU:HB2 | 17:OO:139[A]:LEU:HD22 | 1.77 | 0.66 |
| 17:OO:65[A]:PHE:O | 17:OO:65[A]:PHE:HD1 | 1.73 | 0.66 |
| 83:1:459:ILE:HG22 | 83:1:463:LEU:HG | 1.78 | 0.66 |
| 81:2:1671:G:C6 | 81:2:1672:C:N4 | 2.64 | 0.66 |
| 81:2:811:A:O4' | 81:2:857:G:N2 | 2.29 | 0.66 |
| 1:5:2238:U:C6 | 1:5:2239:A:C8 | 2.84 | 0.66 |
| 1:5:285:A:OP1 | 1:5:306:A:H5'' | 1.94 | 0.66 |
| 83:1:586:ILE:HD12 | 83:1:708:THR:OG1 | 1.93 | 0.66 |
| 81:2:980:U:O2' | 81:2:1122:C:N3 | 2.28 | 0.66 |
| 1:5:2481:C:OP1 | 10:GG:244:LYS:CE | 2.39 | 0.66 |
| 8:EE:126:LYS:HD3 | 8:EE:126:LYS:N | 2.11 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 17:OO:52[A]:LYS:O | 17:OO:52[A]:LYS:HG2 | 1.95 | 0.66 |
| 50:C:169:SER:OG | 50:C:169:SER:O | 2.14 | 0.66 |
| 1:5:1925:G:C2 | 1:5:2056:C:H2' | 2.30 | 0.66 |
| 1:5:2218:G:C5 | 1:5:2219:G:C4 | 2.84 | 0.66 |
| 83:1:589:LYS:HD3 | 83:1:685:ARG:CD | 2.21 | 0.65 |
| 17:OO:11[A]:ASP:OD1 | 17:OO:13[A]:LYS:HB3 | 1.96 | 0.65 |
| 83:1:659:ILE:HD13 | 83:1:693:LEU:HD11 | 1.77 | 0.65 |
| 1:5:1197:G:C5 | 1:5:1198:C:N4 | 2.64 | 0.65 |
| 83:1:638:PRO:HD3 | 83:1:681:MET:HE2 | 1.78 | 0.65 |
| 81:2:366:A:H2' | 81:2:367:U:O4' | 1.96 | 0.65 |
| 81:2:954:A:H2' | 81:2:955:C:O4' | 1.96 | 0.65 |
| 1:5:1186:U:H2' | 1:5:1187:C:O4' | 1.96 | 0.65 |
| 1:5:1925:G:C2 | 1:5:2056:C:C4 | 2.75 | 0.65 |
| 1:5:2167:A:N7 | 1:5:2238:U:N3 | 2.45 | 0.65 |
| 54:G:83:CYS:N | 81:2:161:A:OP1 | 2.29 | 0.65 |
| 83:1:577:SER:OG | 83:1:586:ILE:CB | 2.45 | 0.65 |
| 81:2:987:A:C2 | 81:2:988:U:C2 | 2.85 | 0.65 |
| 1:5:2480:A:C3' | 1:5:2481:C:H4' | 2.26 | 0.65 |
| 17:OO:124[A]:ALA:O | 17:OO:125[A]:LEU:C | 2.33 | 0.65 |
| 83:1:564:ARG:HD2 | 83:1:681:MET:CB | 2.27 | 0.65 |
| 54:G:155:ASP:N | 81:2:78:A:P | 2.70 | 0.65 |
| 14:LL:103:ASN:HB3 | 14:LL:109:LEU:HD21 | 1.79 | 0.65 |
| 17:OO:55[A]:TYR:CE2 | 17:OO:59[A]:LEU:HD13 | 2.31 | 0.65 |
| 83:1:413:ILE:HG23 | 83:1:463:LEU:HD21 | 1.78 | 0.65 |
| 1:5:1554:C:C2' | 1:5:1555:G:H5' | 2.26 | 0.65 |
| 54:G:136:LYS:O | 54:G:175:ILE:HG23 | 1.97 | 0.65 |
| 26:XX:73:MET:N | 26:XX:73:MET:SD | 2.69 | 0.65 |
| 57:J:14:THR:CG2 | 81:2:22:A:O3' | 2.45 | 0.65 |
| 1:5:2236:C:H2' | 1:5:2237:U:C6 | 2.31 | 0.65 |
| 1:5:957:U:C2 | 1:5:958:U:C5 | 2.85 | 0.65 |
| 17:OO:119[A]:VAL:O | 17:OO:119[A]:VAL:CG2 | 2.42 | 0.65 |
| 17:OO:151[A]:GLU:O | 17:OO:154[A]:VAL:N | 2.23 | 0.65 |
| 18:PP:36:ILE:HD11 | 18:PP:95:LEU:HD11 | 1.78 | 0.65 |
| 83:1:380:LEU:CB | 83:1:400:VAL:HA | 2.27 | 0.64 |
| 81:2:1338:C:O2' | 81:2:1340:A:N7 | 2.26 | 0.64 |
| 17:OO:24[A]:VAL:O | 17:OO:28[A]:LEU:HG | 1.97 | 0.64 |
| 83:1:682:ARG:HB2 | 83:1:683:SER:OG | 1.96 | 0.64 |
| 1:5:1925:G:C2 | 1:5:2056:C:C2' | 2.81 | 0.64 |
| 81:2:1131:A:C2 | 81:2:1132:A:C4 | 2.85 | 0.64 |
| 82:4:6104:G:H2' | 82:4:6105:U:O4' | 1.97 | 0.64 |
| 83:1:576:LEU:HD22 | 83:1:586:ILE:O | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:1624:G:H5'' | 1:5:1624:G:H8 | 1.61 | 0.64 |
| 17:OO:193[A]:LYS:HA | 17:OO:193[A]:LYS:CE | 2.15 | 0.64 |
| 18:PP:36:ILE:CD1 | 18:PP:95:LEU:HD11 | 2.27 | 0.64 |
| 83:1:584:ASN:O | 83:1:585:ARG:HG3 | 1.98 | 0.64 |
| 83:1:702:GLY:CA | 83:1:706:ILE:CD1 | 2.44 | 0.64 |
| 81:2:480:A:C6 | 81:2:506:U:C4 | 2.84 | 0.64 |
| 82:4:6127:C:O2 | 82:4:6160:G:N1 | 2.30 | 0.64 |
| 81:2:8:U:C3' | 81:2:9:U:H5' | 2.28 | 0.64 |
| 1:5:1928:A:C2 | 1:5:2053:C:O2' | 2.50 | 0.64 |
| 1:5:1925:G:C4 | 1:5:2056:C:N3 | 2.65 | 0.64 |
| 1:5:2218:G:N3 | 1:5:2219:G:N9 | 2.44 | 0.64 |
| 1:5:2494:G:N7 | 4:AA:67:TYR:OH | 2.29 | 0.64 |
| 12:II:49:CYS:SG | 12:II:51:HIS:CE1 | 2.91 | 0.64 |
| 83:1:694:HIS:N | 83:1:695:ALA:O | 2.29 | 0.64 |
| 50:C:82:LYS:HA | 50:C:83:ASP:HB2 | 1.78 | 0.64 |
| 52:E:9:LEU:HD13 | 52:E:28:ALA:HB3 | 1.80 | 0.64 |
| 17:OO:44[A]:ILE:CD1 | 17:OO:139[A]:LEU:CD1 | 2.72 | 0.64 |
| 17:OO:63[A]:THR:OG1 | 17:OO:70[A]:GLY:HA2 | 1.98 | 0.64 |
| 70:W:55:ASP:O | 70:W:57:ARG:N | 2.31 | 0.64 |
| 1:5:1288:A:C4 | 1:5:1290:G:N7 | 2.66 | 0.64 |
| 1:5:2072:U:H2' | 1:5:2073:A:O4' | 1.98 | 0.64 |
| 1:5:336:A:C2 | 1:5:337:G:C6 | 2.86 | 0.64 |
| 26:XX:105:VAL:HG11 | 26:XX:126:LEU:HD22 | 1.80 | 0.64 |
| 83:1:562:ALA:CB | 83:1:563:TYR:HA | 2.26 | 0.64 |
| 1:5:2167:A:C5 | 1:5:2238:U:N3 | 2.63 | 0.64 |
| 6:CC:349:ILE:CG2 | 6:CC:350:LYS:HG3 | 2.28 | 0.64 |
| 83:1:750:LYS:O | 83:1:751:ARG:CG | 2.44 | 0.63 |
| 1:5:1926:U:N3 | 1:5:2055:G:C4 | 2.66 | 0.63 |
| 1:5:2481:C:C2' | 1:5:2482:U:H6 | 1.99 | 0.63 |
| 1:5:859:A:C2 | 1:5:860:U:C2 | 2.87 | 0.63 |
| 1:5:883:G:N7 | 4:AA:9:ARG:NH2 | 2.46 | 0.63 |
| 17:OO:182[A]:LYS:C | 17:OO:184[A]:ALA:N | 2.50 | 0.63 |
| 83:1:47:SER:HA | 83:1:48:ALA:HB3 | 1.80 | 0.63 |
| 83:1:701:GLY:H | 83:1:704:GLN:HB2 | 1.64 | 0.63 |
| 81:2:391:G:OP1 | 81:2:1727:C:O2' | 2.14 | 0.63 |
| 1:5:2218:G:O2' | 1:5:2219:G:O5' | 2.16 | 0.63 |
| 1:5:2223:U:H2' | 1:5:2224:A:O4' | 1.98 | 0.63 |
| 17:OO:63[A]:THR:O | 17:OO:64[A]:ALA:C | 2.37 | 0.63 |
| 17:OO:98[A]:ALA:O | 17:OO:99[A]:ALA:C | 2.37 | 0.63 |
| 81:2:1592:G:OP2 | 81:2:1594:C:N4 | 2.31 | 0.63 |
| 81:2:886:A:C5 | 81:2:887:U:C4 | 2.86 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 81:2:9:U:O2' | 81:2:11:A:N7 | 2.29 | 0.63 |
| 82:4:6126:C:O2 | 82:4:6161:A:N1 | 2.30 | 0.63 |
| 1:5:2167:A:N9 | 1:5:2238:U:C6 | 2.66 | 0.63 |
| 1:5:2530:A:H1' | 1:5:2531:A:OP1 | 1.99 | 0.63 |
| 1:5:436:A:N6 | 1:5:597:G:C6 | 2.66 | 0.63 |
| 1:5:518:C:O2 | 1:5:518:C:H2' | 1.97 | 0.63 |
| 71:X:7:ARG:HD3 | 81:2:1101:G:OP2 | 1.97 | 0.63 |
| 83:1:685:ARG:HD3 | 83:1:687:ASN:H | 1.63 | 0.63 |
| 81:2:10:G:H2' | 81:2:11:A:C8 | 2.34 | 0.63 |
| 1:5:2107:A:O2' | 1:5:2108:A:OP1 | 2.16 | 0.63 |
| 1:5:2164:C:H2' | 1:5:2165:C:O4' | 1.98 | 0.63 |
| 1:5:2167:A:N1 | 1:5:2238:U:H5 | 1.89 | 0.63 |
| 1:5:674:G:C5 | 1:5:675:C:C4 | 2.87 | 0.63 |
| 5:BB:218:VAL:HG13 | 5:BB:274:HIS:HE1 | 1.63 | 0.63 |
| 17:OO:184[A]:ALA:O | 17:OO:187[A]:GLY:N | 2.32 | 0.63 |
| 83:1:133:GLU:OE1 | 83:1:136:CYS:HB2 | 1.99 | 0.63 |
| 81:2:1044:C:O2 | 81:2:1073:G:C2 | 2.51 | 0.63 |
| 82:4:6134:C:O2' | 82:4:6135:C:O5' | 2.16 | 0.63 |
| 81:2:51:A:N6 | 81:2:439:U:N3 | 2.47 | 0.63 |
| 1:5:1925:G:C2' | 1:5:2055:G:N2 | 2.62 | 0.63 |
| 1:5:2239:A:O2' | 1:5:2240:A:O4' | 2.15 | 0.63 |
| 1:5:2479:U:H2' | 1:5:2480:A:H5' | 1.78 | 0.63 |
| 17:OO:7[A]:VAL:HG13 | 17:OO:8[A]:VAL:H | 1.63 | 0.63 |
| 17:OO:58[A]:TYR:O | 17:OO:59[A]:LEU:C | 2.35 | 0.63 |
| 82:4:6127:C:C2 | 82:4:6160:G:N1 | 2.67 | 0.63 |
| 1:5:2151:A:OP1 | 4:AA:193:ARG:NH2 | 2.32 | 0.63 |
| 1:5:2971:G:N2 | 1:5:2972:C:C2 | 2.67 | 0.63 |
| 1:5:3054:A:H3' | 1:5:3055:A:N7 | 2.14 | 0.63 |
| 3:8:7:U:O2' | 3:8:8:C:H5' | 1.99 | 0.63 |
| 82:4:6189:G:O2' | 87:1:903:6EM:O6 | 2.13 | 0.62 |
| 1:5:2218:G:N2 | 1:5:2219:G:N7 | 2.47 | 0.62 |
| 48:A:90:ALA:HB2 | 48:A:97:PRO:HG3 | 1.81 | 0.62 |
| 13:JJ:82:ARG:HB3 | 13:JJ:112:LEU:HB2 | 1.81 | 0.62 |
| 17:OO:162[A]:LYS:O | 17:OO:163[A]:ALA:C | 2.38 | 0.62 |
| 26:XX:113:LEU:C | 26:XX:113:LEU:HD12 | 2.20 | 0.62 |
| 28:ZZ:46:ILE:HD11 | 28:ZZ:49:TYR:CD2 | 2.34 | 0.62 |
| 83:1:380:LEU:CD1 | 83:1:400:VAL:HG23 | 2.28 | 0.62 |
| 81:2:928:A:C3' | 81:2:929:A:H5' | 2.29 | 0.62 |
| 1:5:1159:U:C4 | 1:5:1288:A:N1 | 2.66 | 0.62 |
| 1:5:2050:A:OP1 | 1:5:2051:U:C5 | 2.51 | 0.62 |
| 1:5:2247:C:C2 | 1:5:2276:G:N2 | 2.67 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:2877:U:H2' | 1:5:2878:A:O4' | 1.98 | 0.62 |
| 1:5:3243:U:H2' | 1:5:3243:U:O2 | 1.97 | 0.62 |
| 5:BB:57:VAL:HG22 | 5:BB:73:VAL:HG22 | 1.81 | 0.62 |
| 17:OO:70[A]:GLY:O | 17:OO:71[A]:PRO:C | 2.37 | 0.62 |
| 63:P:17:TYR:C | 66:S:92:VAL:O | 2.36 | 0.62 |
| 1:5:2167:A:C5 | 1:5:2168:G:C8 | 2.87 | 0.62 |
| 1:5:2218:G:H4' | 1:5:2219:G:OP1 | 1.98 | 0.62 |
| 1:5:2313:U:H2' | 1:5:2314:A:C8 | 2.34 | 0.62 |
| 17:OO:106[A]:PHE:CG | 17:OO:110[A]:PRO:HG3 | 2.33 | 0.62 |
| 81:2:823:G:N2 | 81:2:848:C:C2 | 2.67 | 0.62 |
| 81:2:987:A:H2' | 81:2:988:U:C6 | 2.35 | 0.62 |
| 82:4:6182:A:OP1 | 83:1:585:ARG:NH2 | 2.32 | 0.62 |
| 1:5:1925:G:N3 | 1:5:2056:C:C2' | 2.63 | 0.62 |
| 5:BB:14:LEU:HD23 | 5:BB:17:LEU:HD12 | 1.81 | 0.62 |
| 1:5:1876:C:O2 | 5:BB:240:ARG:NH2 | 2.33 | 0.62 |
| 6:CC:35:VAL:HG21 | 6:CC:244:LEU:HD21 | 1.80 | 0.62 |
| 17:OO:129[A]:ARG:O | 17:OO:130[A]:LEU:C | 2.38 | 0.62 |
| 83:1:727:PRO:CB | 83:1:728:VAL:HA | 2.29 | 0.62 |
| 3:8:9:A:C2 | 3:8:10:A:C6 | 2.86 | 0.62 |
| 17:OO:58[A]:TYR:C | 17:OO:60[A]:ARG:N | 2.52 | 0.62 |
| 83:1:583:HIS:CE1 | 83:1:704:GLN:CB | 2.80 | 0.62 |
| 81:2:628:U:C4 | 81:2:969:A:C6 | 2.85 | 0.62 |
| 81:2:1378:U:O2' | 81:2:1514:A:N1 | 2.32 | 0.62 |
| 82:4:6134:C:O2' | 82:4:6135:C:O4' | 2.16 | 0.62 |
| 17:OO:63[A]:THR:OG1 | 17:OO:70[A]:GLY:CA | 2.48 | 0.62 |
| 17:OO:63[A]:THR:O | 17:OO:65[A]:PHE:N | 2.33 | 0.62 |
| 1:5:1503:C:C2 | 1:5:1560:G:C2 | 2.88 | 0.62 |
| 1:5:2167:A:C8 | 1:5:2238:U:N3 | 2.67 | 0.62 |
| 1:5:887:G:C6 | 4:AA:207:VAL:CG2 | 2.83 | 0.62 |
| 17:OO:4[A]:PHE:C | 17:OO:5[A]:GLU:OE1 | 2.38 | 0.62 |
| 65:R:87:ASP:HB3 | 65:R:88:VAL:HG13 | 1.82 | 0.62 |
| 81:2:1440:U:C4 | 81:2:1441:U:C4 | 2.87 | 0.62 |
| 61:N:46:THR:OG1 | 61:N:49:GLN:NE2 | 2.33 | 0.62 |
| 17:OO:120[A]:VAL:O | 17:OO:122[A]:PRO:CD | 2.44 | 0.62 |
| 17:OO:28[A]:LEU:C | 17:OO:30[A]:ASN:H | 2.02 | 0.62 |
| 83:1:638:PRO:HD3 | 83:1:681:MET:CE | 2.26 | 0.61 |
| 81:2:887:U:O2' | 81:2:987:A:O2' | 2.14 | 0.61 |
| 1:5:2235:U:H2' | 1:5:2236:C:C6 | 2.34 | 0.61 |
| 54:G:155:ASP:N | 81:2:77:U:O3' | 2.32 | 0.61 |
| 1:5:248:U:O2 | 1:5:248:U:H2' | 2.00 | 0.61 |
| 1:5:502:G:C2 | 1:5:535:C:C2 | 2.88 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------------|--------------------------|-------------------|
| 83:1:696:ASP:HB2 | 83:1:698:ILE:HG23 | 1.80 | 0.61 |
| 1:5:2280:G:H4' | 1:5:2285:G:H5'' | 1.82 | 0.61 |
| 83:1:378:LEU:HD23 | 83:1:405:VAL:HG13 | 1.81 | 0.61 |
| 1:5:2218:G:H3' | 1:5:2218:G:P | 2.40 | 0.61 |
| 1:5:3243:U:O2 | 1:5:3243:U:C2' | 2.48 | 0.61 |
| 17:OO:113[A]:TYR:C | 17:OO:115[A]:LYS:H | 2.04 | 0.61 |
| 17:OO:145[A]:SER:C | 17:OO:146[A]:VAL:CG1 | 2.66 | 0.61 |
| 82:4:6200:A:H4' | 82:4:6201:C:H5'' | 1.82 | 0.61 |
| 1:5:2217:C:H3' | 1:5:2218:G:H5'' | 1.60 | 0.61 |
| 1:5:292:U:H2' | 1:5:293:C:O4' | 2.00 | 0.61 |
| 51:D:186:VAL:HG12 | 51:D:188:ILE:HD11 | 1.82 | 0.61 |
| 17:OO:197[A]:LEU:C | 17:OO:199[A]:TYR:N | 2.52 | 0.61 |
| 70:W:77:PRO:HG2 | 70:W:79:PHE:CZ | 2.36 | 0.61 |
| 17:OO:143[A]:SER:O | 17:OO:146[A]:VAL:N | 2.34 | 0.61 |
| 5:BB:87:VAL:HG22 | 5:BB:110:LEU:HD23 | 1.81 | 0.61 |
| 81:2:1046:G:N2 | 81:2:1071:C:C2 | 2.69 | 0.61 |
| 1:5:1333:G:H2' | 1:5:1334:A:C8 | 2.36 | 0.61 |
| 51:D:134:CYS:SG | 51:D:135:GLU:N | 2.73 | 0.61 |
| 17:OO:49[A]:PHE:O | 17:OO:50[A]:ARG:O | 2.19 | 0.61 |
| 1:5:1074:A:H3' | 1:5:1075:G:H5' | 1.83 | 0.61 |
| 1:5:2218:G:H5'' | 1:5:2242:G:C8 | 2.36 | 0.61 |
| 1:5:426:G:C2 | 1:5:607:C:O2 | 2.54 | 0.61 |
| 17:OO:49[A]:PHE:O | 17:OO:49[A]:PHE:CD1 | 2.54 | 0.61 |
| 1:5:2663:A:N1 | 1:5:2727:U:O4 | 2.33 | 0.60 |
| 1:5:426:G:C6 | 1:5:427:C:N4 | 2.69 | 0.60 |
| 1:5:533:G:C6 | 1:5:534:C:C4 | 2.89 | 0.60 |
| 3:8:115:C:H2' | 3:8:116:G:O4' | 2.00 | 0.60 |
| 1:5:1357:A:O4' | 6:CC:141:ARG:NH2 | 2.33 | 0.60 |
| 17:OO:86[A]:ARG:HA | 17:OO:100[A]:LEU:HD11 | 1.83 | 0.60 |
| 83:1:519:LEU:O | 83:1:519:LEU:HD12 | 2.01 | 0.60 |
| 81:2:886:A:N1 | 81:2:925:A:N1 | 2.49 | 0.60 |
| 82:4:6189:G:H5' | 83:1:582:LYS:HE2 | 1.84 | 0.60 |
| 82:4:6178:U:O4 | 82:4:6198:A:N1 | 2.34 | 0.60 |
| 1:5:103:G:OP1 | 14:LL:70:ARG:NH2 | 2.34 | 0.60 |
| 1:5:2106:U:OP2 | 1:5:2111:A:N6 | 2.34 | 0.60 |
| 2:7:113:C:H2' | 2:7:114:U:O4' | 2.01 | 0.60 |
| 83:1:576:LEU:CD2 | 83:1:587:TYR:CE1 | 2.81 | 0.60 |
| 83:1:701:GLY:HA3 | 83:1:705:ILE:H | 1.66 | 0.60 |
| 81:2:605:A:H4' | 81:2:606:G:H5'' | 1.83 | 0.60 |
| 82:4:6195:G:O2' | 82:4:6196:A:C8 | 2.44 | 0.60 |
| 1:5:173:G:C2 | 1:5:174:C:C2 | 2.89 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:5:2235:U:C2' | 1:5:2236:C:C5 | 2.85 | 0.60 |
| 1:5:594:A:OP1 | 18:PP:167:ARG:NH2 | 2.34 | 0.60 |
| 83:1:577:SER:O | 83:1:578:LYS:HG3 | 2.02 | 0.60 |
| 1:5:2062:A:C8 | 1:5:2063:C:H1' | 2.37 | 0.60 |
| 1:5:2235:U:C2' | 1:5:2236:C:C6 | 2.84 | 0.60 |
| 17:OO:122[A]:PRO:O | 17:OO:124[A]:ALA:N | 2.34 | 0.60 |
| 83:1:579:SER:CB | 83:1:708:THR:HB | 2.28 | 0.60 |
| 81:2:1462:G:N1 | 81:2:1463:C:C4 | 2.70 | 0.60 |
| 1:5:1792:A:H2' | 1:5:1793:U:O4' | 2.01 | 0.60 |
| 72:Y:40:LEU:HD13 | 72:Y:60:PHE:CZ | 2.37 | 0.60 |
| 67:T:38:LYS:NZ | 81:2:1562:U:OP1 | 2.23 | 0.60 |
| 1:5:3210:G:OP1 | 17:OO:164[A]:ARG:NH2 | 2.35 | 0.60 |
| 1:5:2506:U:P | 49:B:226:GLY:O | 2.59 | 0.60 |
| 2:7:8:G:P | 7:DD:33:ARG:HH12 | 2.23 | 0.60 |
| 53:F:70:ILE:HD13 | 53:F:90:PRO:HG3 | 1.84 | 0.60 |
| 17:OO:154[A]:VAL:O | 17:OO:154[A]:VAL:CG1 | 2.49 | 0.60 |
| 83:1:685:ARG:HG2 | 83:1:685:ARG:NH1 | 2.16 | 0.60 |
| 83:1:72:SER:CB | 83:1:73:THR:HA | 2.32 | 0.60 |
| 1:5:1926:U:O2 | 1:5:2055:G:H1' | 2.02 | 0.60 |
| 1:5:2332:A:H2' | 1:5:2333:G:O4' | 2.01 | 0.60 |
| 5:BB:254:ALA:O | 5:BB:256:HIS:N | 2.34 | 0.60 |
| 17:OO:130[A]:LEU:O | 17:OO:131[A]:LYS:C | 2.40 | 0.60 |
| 17:OO:23[A]:THR:O | 17:OO:24[A]:VAL:C | 2.39 | 0.60 |
| 83:1:584:ASN:O | 83:1:585:ARG:CG | 2.50 | 0.60 |
| 6:CC:349:ILE:HG13 | 6:CC:350:LYS:HA | 1.83 | 0.60 |
| 11:HH:4:ILE:HD11 | 21:SS:150:PHE:CD1 | 2.37 | 0.60 |
| 1:5:640:C:H1' | 14:LL:10:LEU:HD21 | 1.83 | 0.60 |
| 18:PP:22:LEU:HD12 | 18:PP:146:ILE:HD12 | 1.84 | 0.60 |
| 83:1:413:ILE:CG2 | 83:1:463:LEU:CD2 | 2.80 | 0.60 |
| 81:2:1671:G:H2' | 81:2:1672:C:C6 | 2.37 | 0.60 |
| 8:EE:128:GLU:O | 8:EE:129:ILE:CB | 2.47 | 0.60 |
| 14:LL:10:LEU:HD23 | 19:QQ:166:GLN:NE2 | 2.17 | 0.60 |
| 17:OO:122[A]:PRO:C | 17:OO:124[A]:ALA:H | 2.04 | 0.60 |
| 17:OO:55[A]:TYR:O | 17:OO:58[A]:TYR:N | 2.25 | 0.60 |
| 81:2:1752:A:HO2' | 81:2:1753:A:P | 2.21 | 0.60 |
| 81:2:363:G:C2 | 81:2:380:C:C2 | 2.90 | 0.60 |
| 54:G:155:ASP:N | 81:2:78:A:C5' | 2.59 | 0.60 |
| 83:1:698:ILE:HG22 | 83:1:699:HIS:CB | 2.32 | 0.59 |
| 81:2:1440:U:H2' | 81:2:1441:U:O4' | 2.02 | 0.59 |
| 1:5:2052:G:H5'' | 1:5:2053:C:OP1 | 2.01 | 0.59 |
| 17:OO:127[A]:VAL:O | 17:OO:127[A]:VAL:CG1 | 2.47 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 83:1:687:ASN:HB3 | 83:1:688:ILE:HA | 1.83 | 0.59 |
| 81:2:10:G:H8 | 81:2:1631:A:O2' | 1.85 | 0.59 |
| 14:LL:74:GLY:O | 14:LL:101:ARG:NH1 | 2.35 | 0.59 |
| 17:OO:13[A]:LYS:HG2 | 17:OO:14[A]:GLY:N | 2.17 | 0.59 |
| 83:1:587:TYR:CD2 | 83:1:690:ASP:C | 2.76 | 0.59 |
| 83:1:687:ASN:CB | 83:1:688:ILE:HA | 2.32 | 0.59 |
| 81:2:12:U:H2' | 81:2:13:C:C6 | 2.37 | 0.59 |
| 82:4:6199:A:H2' | 82:4:6200:A:H5' | 1.83 | 0.59 |
| 1:5:2234:C:H2' | 1:5:2235:U:C6 | 2.36 | 0.59 |
| 14:LL:4:SER:HB3 | 14:LL:5:LYS:HD2 | 1.84 | 0.59 |
| 17:OO:9[A]:VAL:CG1 | 17:OO:118[A]:ARG:HB3 | 2.32 | 0.59 |
| 17:OO:12[A]:GLY:O | 17:OO:13[A]:LYS:C | 2.38 | 0.59 |
| 17:OO:182[A]:LYS:HA | 17:OO:185[A]:THR:HG22 | 1.83 | 0.59 |
| 17:OO:49[A]:PHE:CD1 | 17:OO:49[A]:PHE:C | 2.75 | 0.59 |
| 17:OO:63[A]:THR:H | 17:OO:70[A]:GLY:HA3 | 1.67 | 0.59 |
| 1:5:2352:C:OP2 | 17:OO:86[A]:ARG:NH2 | 2.35 | 0.59 |
| 17:OO:93[A]:THR:O | 17:OO:96[A]:GLY:N | 2.35 | 0.59 |
| 82:4:6121:A:N6 | 82:4:6158:A:C2 | 2.70 | 0.59 |
| 1:5:1197:G:C4 | 1:5:1198:C:C4 | 2.91 | 0.59 |
| 1:5:922:A:C4 | 1:5:1340:A:C2 | 2.90 | 0.59 |
| 1:5:2163:G:N2 | 1:5:2164:C:C2 | 2.70 | 0.59 |
| 1:5:2249:A:C2' | 1:5:2250:A:H5' | 2.31 | 0.59 |
| 1:5:3055:A:C5' | 1:5:3055:A:H8 | 2.14 | 0.59 |
| 1:5:3220:G:H2' | 1:5:3221:G:O4' | 2.03 | 0.59 |
| 1:5:844:C:H3' | 1:5:845:U:H4' | 1.84 | 0.59 |
| 17:OO:42[A]:LEU:N | 17:OO:42[A]:LEU:CD1 | 2.62 | 0.59 |
| 63:P:17:TYR:N | 66:S:92:VAL:O | 2.35 | 0.59 |
| 83:1:54:ALA:HB1 | 83:1:55:ARG:HG2 | 1.84 | 0.59 |
| 82:4:6134:C:O2' | 82:4:6135:C:C5' | 2.50 | 0.59 |
| 1:5:2218:G:H3' | 1:5:2218:G:OP2 | 2.03 | 0.59 |
| 6:CC:350:LYS:HD3 | 9:FF:68:ALA:CB | 2.33 | 0.59 |
| 51:D:162:GLN:O | 51:D:164:VAL:N | 2.36 | 0.59 |
| 24:VV:34:LEU:HD21 | 24:VV:102:ILE:HG22 | 1.84 | 0.59 |
| 83:1:371:ASN:HB3 | 83:1:373:ASP:OD1 | 2.01 | 0.59 |
| 83:1:591:GLU:HB3 | 83:1:592:PRO:C | 2.22 | 0.59 |
| 81:2:566:A:N1 | 81:2:582:C:H1' | 2.18 | 0.59 |
| 1:5:1107:A:C2 | 1:5:1108:C:C4 | 2.91 | 0.59 |
| 1:5:1923:G:C6 | 1:5:2057:A:C2 | 2.89 | 0.59 |
| 54:G:5:ILE:HD12 | 54:G:16:ILE:HD13 | 1.83 | 0.59 |
| 83:1:164:LEU:HD22 | 83:1:285:PHE:CD2 | 2.38 | 0.59 |
| 83:1:405:VAL:HA | 83:1:406:LYS:HB3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 83:1:685:ARG:HH11 | 83:1:685:ARG:CG | 2.15 | 0.59 |
| 1:5:2981:U:H2' | 1:5:2982:U:C6 | 2.38 | 0.59 |
| 17:OO:188[A]:THR:O | 17:OO:189[A]:GLU:O | 2.21 | 0.59 |
| 81:2:1440:U:H5' | 81:2:1445:C:N4 | 2.16 | 0.59 |
| 1:5:2238:U:H2' | 1:5:2239:A:C5' | 2.33 | 0.59 |
| 1:5:931:U:O2' | 1:5:932:C:H5' | 2.02 | 0.59 |
| 11:HH:27:VAL:HG12 | 11:HH:82:VAL:HG11 | 1.83 | 0.59 |
| 17:OO:139[A]:LEU:C | 17:OO:141[A]:LYS:N | 2.56 | 0.59 |
| 17:OO:55[A]:TYR:C | 17:OO:57[A]:ASP:N | 2.50 | 0.59 |
| 1:5:2055:G:N3 | 1:5:2056:C:C2 | 2.71 | 0.59 |
| 1:5:2247:C:N3 | 1:5:2276:G:C2 | 2.70 | 0.59 |
| 1:5:674:G:C6 | 1:5:675:C:N3 | 2.70 | 0.59 |
| 3:8:118:C:C2 | 3:8:136:G:N2 | 2.71 | 0.59 |
| 4:AA:57:PRO:HD2 | 4:AA:170:ALA:HB3 | 1.84 | 0.59 |
| 59:L:78:THR:HG22 | 59:L:84:ILE:HD11 | 1.85 | 0.59 |
| 21:SS:79:VAL:HG13 | 21:SS:121:ILE:HG23 | 1.85 | 0.59 |
| 1:5:2218:G:C8 | 1:5:2219:G:O4' | 2.56 | 0.59 |
| 1:5:2218:G:C6 | 1:5:2219:G:C2 | 2.90 | 0.59 |
| 1:5:803:G:C2 | 1:5:834:C:C2 | 2.91 | 0.59 |
| 9:FF:166:VAL:HG21 | 9:FF:178:VAL:HG22 | 1.85 | 0.59 |
| 63:P:19:GLY:N | 66:S:93:ASN:N | 2.51 | 0.59 |
| 71:X:7:ARG:NH2 | 81:2:1099:G:O4' | 2.35 | 0.58 |
| 81:2:864:A:N1 | 81:2:964:U:C5 | 2.71 | 0.58 |
| 1:5:2050:A:C2' | 1:5:2051:U:OP1 | 2.51 | 0.58 |
| 1:5:2167:A:H2' | 1:5:2168:G:O5' | 2.03 | 0.58 |
| 1:5:78:U:O2 | 1:5:78:U:C2' | 2.50 | 0.58 |
| 17:OO:99[A]:ALA:C | 17:OO:101[A]:GLU:H | 2.06 | 0.58 |
| 17:OO:190[A]:VAL:C | 17:OO:192[A]:GLU:N | 2.54 | 0.58 |
| 81:2:1349:G:C2 | 81:2:1374:C:O2 | 2.56 | 0.58 |
| 81:2:385:G:O2' | 81:2:424:A:N1 | 2.28 | 0.58 |
| 81:2:478:C:H2' | 81:2:479:G:O4' | 2.03 | 0.58 |
| 1:5:891:A:OP1 | 1:5:894:C:N4 | 2.35 | 0.58 |
| 17:OO:16[A]:LEU:HD21 | 17:OO:130[A]:LEU:HD22 | 1.85 | 0.58 |
| 17:OO:143[A]:SER:O | 17:OO:144[A]:THR:C | 2.40 | 0.58 |
| 81:2:1462:G:N2 | 81:2:1463:C:C2 | 2.72 | 0.58 |
| 81:2:969:A:N6 | 81:2:970:A:C5 | 2.72 | 0.58 |
| 1:5:312:C:O2 | 1:5:2746:G:C2 | 2.56 | 0.58 |
| 1:5:3296:G:C2 | 1:5:3347:C:C2 | 2.91 | 0.58 |
| 1:5:340:C:C2 | 3:8:25:G:N2 | 2.71 | 0.58 |
| 4:AA:196:TRP:CE3 | 4:AA:197:PRO:CD | 2.86 | 0.58 |
| 17:OO:11[A]:ASP:OD1 | 17:OO:13[A]:LYS:CB | 2.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 17:OO:75[A]:ARG:CD | 17:OO:146[A]:VAL:O | 2.51 | 0.58 |
| 1:5:1083:A:P | 14:LL:5:LYS:NZ | 2.75 | 0.58 |
| 1:5:2852:C:O2 | 1:5:2907:G:C2 | 2.56 | 0.58 |
| 1:5:3274:U:H2' | 1:5:3275:A:H5'' | 1.83 | 0.58 |
| 23:UU:80:THR:HG21 | 23:UU:95:PHE:CE1 | 2.38 | 0.58 |
| 82:4:6121:A:N6 | 82:4:6158:A:H2 | 2.01 | 0.58 |
| 1:5:1033:A:C2 | 1:5:1069:A:C5 | 2.92 | 0.58 |
| 1:5:2050:A:OP1 | 1:5:2051:U:O4 | 2.21 | 0.58 |
| 1:5:2480:A:N6 | 1:5:2481:C:C4 | 2.71 | 0.58 |
| 1:5:2704:A:OP1 | 22:TT:92:ARG:NH1 | 2.36 | 0.58 |
| 10:GG:142:ILE:HD11 | 10:GG:150:VAL:HG21 | 1.84 | 0.58 |
| 83:1:683:SER:H | 83:1:684:VAL:HG23 | 1.67 | 0.58 |
| 81:2:1086:A:H2' | 81:2:1087:A:C8 | 2.39 | 0.58 |
| 1:5:2237:U:C3' | 1:5:2238:U:H5' | 2.34 | 0.58 |
| 1:5:2239:A:C2' | 1:5:2240:A:H8 | 2.08 | 0.58 |
| 1:5:2237:U:C2 | 1:5:2241:G:O6 | 2.56 | 0.58 |
| 11:HH:90:LEU:CD2 | 11:HH:181:VAL:HG22 | 2.33 | 0.58 |
| 83:1:591:GLU:HB3 | 83:1:592:PRO:CA | 2.32 | 0.58 |
| 1:5:1800:U:H2' | 1:5:1801:C:C6 | 2.38 | 0.58 |
| 1:5:422:A:N1 | 1:5:2331:C:O2' | 2.31 | 0.58 |
| 83:1:694:HIS:H | 83:1:695:ALA:CA | 2.16 | 0.58 |
| 81:2:977:A:H2' | 81:2:978:A:O4' | 2.04 | 0.58 |
| 1:5:1925:G:C5 | 1:5:2057:A:C4 | 2.91 | 0.58 |
| 1:5:2218:G:H2' | 1:5:2219:G:C8 | 2.39 | 0.58 |
| 1:5:343:U:O4' | 6:CC:95:ARG:NH2 | 2.37 | 0.58 |
| 1:5:420:G:H4' | 1:5:421:G:OP1 | 2.03 | 0.58 |
| 1:5:3054:A:H4' | 5:BB:366:GLY:HA2 | 1.85 | 0.58 |
| 1:5:1159:U:N3 | 1:5:1288:A:N6 | 2.50 | 0.58 |
| 1:5:324:A:C6 | 1:5:325:A:N6 | 2.72 | 0.58 |
| 1:5:916:C:H2' | 1:5:917:U:C6 | 2.39 | 0.58 |
| 9:FF:135:TYR:CE2 | 9:FF:230:GLU:HA | 2.39 | 0.58 |
| 1:5:2911:G:O2' | 5:BB:254:ALA:HB1 | 2.03 | 0.58 |
| 5:BB:232:ARG:NH1 | 5:BB:268:GLY:O | 2.37 | 0.58 |
| 1:5:3211:A:N1 | 17:OO:109[A]:VAL:N | 2.51 | 0.58 |
| 17:OO:139[A]:LEU:O | 17:OO:141[A]:LYS:C | 2.42 | 0.58 |
| 17:OO:49[A]:PHE:CE1 | 17:OO:53[A]:LEU:HG | 2.39 | 0.58 |
| 83:1:659:ILE:CD1 | 83:1:693:LEU:HD21 | 2.34 | 0.57 |
| 82:4:6200:A:H4' | 82:4:6201:C:C5' | 2.33 | 0.57 |
| 1:5:1923:G:N1 | 1:5:2057:A:H2 | 2.00 | 0.57 |
| 1:5:2238:U:C2' | 1:5:2239:A:C5' | 2.82 | 0.57 |
| 1:5:2667:G:N2 | 1:5:2724:C:C2 | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:5:599:U:H2' | 1:5:600:U:O4' | 2.03 | 0.57 |
| 17:OO:43[A]:ASN:OD1 | 17:OO:126[A]:ARG:NH1 | 2.36 | 0.57 |
| 27:YY:70:VAL:HG22 | 27:YY:82:VAL:HA | 1.85 | 0.57 |
| 83:1:685:ARG:HD3 | 83:1:687:ASN:N | 2.19 | 0.57 |
| 81:2:1292:U:O4 | 81:2:1293:G:C4 | 2.56 | 0.57 |
| 82:4:6120:U:O2' | 82:4:6121:A:OP1 | 2.21 | 0.57 |
| 1:5:1924:C:C4 | 1:5:2055:G:C6 | 2.92 | 0.57 |
| 5:BB:86:VAL:HG13 | 5:BB:160:VAL:HG13 | 1.86 | 0.57 |
| 6:CC:349:ILE:CG1 | 6:CC:350:LYS:HA | 2.33 | 0.57 |
| 6:CC:350:LYS:HD2 | 6:CC:350:LYS:H | 1.68 | 0.57 |
| 1:5:336:A:H1' | 6:CC:48:GLN:HE22 | 1.68 | 0.57 |
| 57:J:170:GLY:HA3 | 81:2:510:A:C3' | 2.34 | 0.57 |
| 81:2:332:A:H2' | 81:2:333:G:C8 | 2.39 | 0.57 |
| 53:F:203:ALA:HA | 53:F:213:ILE:HD11 | 1.86 | 0.57 |
| 24:VV:37:MET:HE1 | 24:VV:73:VAL:HG22 | 1.85 | 0.57 |
| 71:X:11:SER:O | 71:X:13:ARG:N | 2.36 | 0.57 |
| 83:1:381:TYR:OH | 83:1:466:THR:HB | 2.04 | 0.57 |
| 82:4:6189:G:OP1 | 83:1:582:LYS:NZ | 2.37 | 0.57 |
| 83:1:583:HIS:HE1 | 83:1:704:GLN:CB | 2.17 | 0.57 |
| 83:1:680:GLU:HG2 | 83:1:681:MET:HB2 | 1.87 | 0.57 |
| 82:4:6188:G:H4' | 83:1:696:ASP:OD2 | 2.05 | 0.57 |
| 1:5:1753:G:H2' | 1:5:1754:C:O4' | 2.05 | 0.57 |
| 1:5:3243:U:O2' | 1:5:3244:G:C4' | 2.52 | 0.57 |
| 83:1:694:HIS:H | 83:1:695:ALA:C | 2.07 | 0.57 |
| 83:1:698:ILE:HG21 | 83:1:699:HIS:CD2 | 2.29 | 0.57 |
| 70:W:8:ALA:HA | 70:W:74:VAL:HG21 | 1.87 | 0.57 |
| 83:1:577:SER:OG | 83:1:586:ILE:CA | 2.52 | 0.57 |
| 81:2:921:G:H2' | 81:2:922:A:C8 | 2.39 | 0.57 |
| 1:5:2630:G:H2' | 1:5:2631:A:C8 | 2.39 | 0.57 |
| 5:BB:215:ILE:HD12 | 5:BB:282:VAL:HG21 | 1.85 | 0.57 |
| 9:FF:87:LYS:HD2 | 9:FF:217:PHE:CE1 | 2.38 | 0.57 |
| 17:OO:190[A]:VAL:C | 17:OO:192[A]:GLU:H | 2.08 | 0.57 |
| 1:5:3154:A:OP1 | 21:SS:154:HIS:ND1 | 2.37 | 0.57 |
| 24:VV:15:LEU:HD23 | 24:VV:53:SER:HB3 | 1.86 | 0.57 |
| 83:1:577:SER:OG | 83:1:586:ILE:N | 2.35 | 0.57 |
| 1:5:148:G:OP2 | 16:NN:4:TYR:OH | 2.20 | 0.57 |
| 1:5:2850:U:H2' | 1:5:2851:U:O4' | 2.04 | 0.57 |
| 1:5:3127:C:H2' | 1:5:3128:C:C6 | 2.40 | 0.57 |
| 17:OO:28[A]:LEU:HD11 | 17:OO:103[A]:LEU:HB2 | 1.87 | 0.57 |
| 1:5:1328:G:C2 | 1:5:1329:C:C2 | 2.92 | 0.57 |
| 1:5:2228:A:H1' | 1:5:2229:U:H2' | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 1:5:2529:C:H2' | 1:5:2529:C:O2 | 2.05 | 0.57 |
| 12:II:52:LEU:HG | 12:II:165:ILE:HG22 | 1.86 | 0.57 |
| 17:OO:126[A]:ARG:HG3 | 17:OO:130[A]:LEU:CD2 | 2.29 | 0.57 |
| 17:OO:175[A]:TYR:O | 17:OO:179[A]:VAL:HG23 | 2.05 | 0.57 |
| 71:X:96:VAL:HA | 71:X:127:VAL:HG11 | 1.87 | 0.57 |
| 83:1:584:ASN:C | 83:1:585:ARG:HG3 | 2.26 | 0.57 |
| 83:1:89:ILE:HG21 | 83:1:93:THR:HG21 | 1.86 | 0.57 |
| 1:5:1092:U:H2' | 1:5:1093:U:C6 | 2.39 | 0.57 |
| 1:5:1196:A:H3' | 1:5:1197:G:H5' | 1.87 | 0.57 |
| 1:5:1209:C:H2' | 1:5:1210:C:O4' | 2.05 | 0.57 |
| 81:2:1044:C:N3 | 81:2:1073:G:C6 | 2.72 | 0.57 |
| 81:2:823:G:C2 | 81:2:848:C:N3 | 2.73 | 0.57 |
| 1:5:413:U:H2' | 1:5:414:U:C6 | 2.40 | 0.57 |
| 15:MM:55:ARG:NH1 | 21:SS:70:THR:O | 2.37 | 0.57 |
| 83:1:735:CYS:SG | 83:1:740:VAL:HG11 | 2.45 | 0.56 |
| 81:2:1103:U:H2' | 81:2:1104:C:O4' | 2.04 | 0.56 |
| 81:2:1464:G:N2 | 81:2:1465:C:C2 | 2.73 | 0.56 |
| 1:5:2418:A:H2' | 1:5:2419:G:O4' | 2.05 | 0.56 |
| 11:HH:90:LEU:HB2 | 11:HH:144:ILE:HG23 | 1.85 | 0.56 |
| 1:5:2480:A:H3' | 1:5:2481:C:H4' | 1.84 | 0.56 |
| 1:5:533:G:C2 | 1:5:534:C:C2 | 2.93 | 0.56 |
| 17:OO:31[A]:GLY:HA2 | 17:OO:102[A]:ARG:CZ | 2.35 | 0.56 |
| 1:5:2225:A:N6 | 1:5:2229:U:H1' | 2.19 | 0.56 |
| 1:5:2167:A:C1' | 1:5:2238:U:C1' | 2.83 | 0.56 |
| 17:OO:142[A]:LEU:O | 17:OO:143[A]:SER:C | 2.44 | 0.56 |
| 17:OO:171[A]:LYS:HZ3 | 17:OO:171[A]:LYS:HB3 | 1.68 | 0.56 |
| 54:G:154:ARG:H | 81:2:78:A:C5' | 2.18 | 0.56 |
| 1:5:1925:G:O6 | 1:5:2057:A:C4 | 2.58 | 0.56 |
| 1:5:282:G:H4' | 1:5:283:G:O5' | 2.06 | 0.56 |
| 6:CC:156:LEU:HD12 | 6:CC:156:LEU:C | 2.25 | 0.56 |
| 59:L:86:ILE:HD13 | 59:L:125:VAL:HG11 | 1.87 | 0.56 |
| 60:M:55:LEU:HD22 | 60:M:79:LEU:HD22 | 1.87 | 0.56 |
| 17:OO:47[A]:GLU:O | 17:OO:49[A]:PHE:N | 2.38 | 0.56 |
| 27:YY:56:VAL:CG2 | 27:YY:104:VAL:HG13 | 2.35 | 0.56 |
| 81:2:1014:U:C6 | 81:2:1015:C:N3 | 2.74 | 0.56 |
| 82:4:6133:G:H2' | 82:4:6134:C:C5 | 2.41 | 0.56 |
| 1:5:1926:U:C2 | 1:5:2055:G:N3 | 2.73 | 0.56 |
| 1:5:2149:G:C6 | 1:5:2150:C:N4 | 2.73 | 0.56 |
| 10:GG:49:VAL:CG2 | 10:GG:51:TRP:CE2 | 2.88 | 0.56 |
| 19:QQ:67:ILE:HG23 | 19:QQ:81:ILE:HD12 | 1.88 | 0.56 |
| 83:1:20:ARG:NH2 | 83:1:342:LEU:HD13 | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 83:1:371:ASN:O | 83:1:372:CYS:CB | 2.54 | 0.56 |
| 81:2:899:A:HO2' | 81:2:915:U:HO2' | 1.53 | 0.56 |
| 1:5:1122:U:H5'' | 1:5:1123:G:OP2 | 2.05 | 0.56 |
| 1:5:1923:G:N1 | 1:5:1925:G:N7 | 2.53 | 0.56 |
| 1:5:3120:U:C5 | 1:5:3363:G:C6 | 2.94 | 0.56 |
| 62:O:19:ILE:HG13 | 62:O:28:VAL:HG13 | 1.87 | 0.56 |
| 17:OO:142[A]:LEU:O | 17:OO:145[A]:SER:N | 2.34 | 0.56 |
| 17:OO:182[A]:LYS:O | 17:OO:183[A]:SER:C | 2.44 | 0.56 |
| 17:OO:50[A]:ARG:HG2 | 17:OO:50[A]:ARG:HH11 | 1.70 | 0.56 |
| 24:VV:13:ILE:HD12 | 24:VV:54:LEU:HB3 | 1.88 | 0.56 |
| 83:1:157:ILE:HD12 | 83:1:211:PHE:CD1 | 2.39 | 0.56 |
| 83:1:204:PRO:HB2 | 83:1:245:TRP:CD2 | 2.41 | 0.56 |
| 1:5:1678:C:C2 | 1:5:1705:G:C2 | 2.94 | 0.56 |
| 1:5:1678:C:C2 | 1:5:1705:G:N2 | 2.74 | 0.56 |
| 1:5:2480:A:C6 | 1:5:2481:C:C4 | 2.92 | 0.56 |
| 1:5:3055:A:H2' | 1:5:3056:G:O4' | 2.05 | 0.56 |
| 1:5:3224:G:H2' | 1:5:3225:C:O4' | 2.06 | 0.56 |
| 1:5:601:A:H2' | 1:5:602:A:H8 | 1.65 | 0.56 |
| 17:OO:190[A]:VAL:O | 17:OO:191[A]:SER:C | 2.43 | 0.56 |
| 69:V:60:ARG:HA | 69:V:65:ALA:HB2 | 1.87 | 0.56 |
| 83:1:695:ALA:CA | 83:1:700:ARG:HH11 | 2.13 | 0.56 |
| 1:5:1068:G:H4' | 1:5:1069:A:O5' | 2.06 | 0.56 |
| 1:5:1083:A:P | 14:LL:5:LYS:HZ1 | 2.29 | 0.56 |
| 17:OO:14[A]:GLY:O | 17:OO:15[A]:HIS:O | 2.23 | 0.56 |
| 83:1:584:ASN:HB3 | 83:1:693:LEU:HA | 1.86 | 0.56 |
| 49:B:116:LYS:HG2 | 81:2:931:U:OP2 | 2.06 | 0.56 |
| 81:2:8:U:C2' | 81:2:9:U:H5' | 2.36 | 0.56 |
| 1:5:1207:G:N2 | 1:5:1215:A:OP1 | 2.38 | 0.56 |
| 1:5:1288:A:O2' | 1:5:1289:A:H3' | 2.05 | 0.56 |
| 1:5:2438:G:C2 | 1:5:2439:C:N3 | 2.74 | 0.56 |
| 1:5:2864:A:H5'' | 1:5:2864:A:C8 | 2.41 | 0.56 |
| 1:5:595:A:C6 | 1:5:596:U:C5 | 2.93 | 0.56 |
| 1:5:970:G:C6 | 1:5:971:C:N4 | 2.74 | 0.56 |
| 17:OO:42[A]:LEU:H | 17:OO:42[A]:LEU:HD13 | 1.69 | 0.56 |
| 17:OO:77[A]:PRO:HD2 | 17:OO:148[A]:TRP:CD1 | 2.41 | 0.56 |
| 83:1:387:PRO:HA | 83:1:394:PHE:HB2 | 1.88 | 0.56 |
| 83:1:695:ALA:HA | 83:1:700:ARG:HH12 | 1.67 | 0.56 |
| 81:2:207:U:H2' | 81:2:208:U:C6 | 2.41 | 0.56 |
| 81:2:284:G:N2 | 81:2:285:C:C2 | 2.74 | 0.56 |
| 1:5:2413:C:O2 | 1:5:2413:C:C2' | 2.54 | 0.56 |
| 1:5:2480:A:H2' | 1:5:2481:C:H4' | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:5:3224:G:C6 | 1:5:3225:C:N3 | 2.74 | 0.56 |
| 53:F:64:ILE:HG23 | 53:F:91:ILE:HG21 | 1.88 | 0.56 |
| 64:Q:83:GLN:HE22 | 64:Q:119:ALA:HA | 1.71 | 0.56 |
| 22:TT:11:THR:O | 22:TT:13:TYR:N | 2.39 | 0.56 |
| 83:1:698:ILE:CB | 83:1:699:HIS:CA | 2.83 | 0.56 |
| 81:2:1349:G:C6 | 81:2:1374:C:N3 | 2.74 | 0.56 |
| 81:2:46:A:N1 | 81:2:431:G:O2' | 2.30 | 0.56 |
| 1:5:2234:C:H2' | 1:5:2235:U:H6 | 1.69 | 0.56 |
| 1:5:2540:A:C2' | 1:5:2540:A:N3 | 2.69 | 0.56 |
| 1:5:2949:U:O2' | 1:5:2950:A:H5' | 2.06 | 0.56 |
| 3:8:24:G:H2' | 3:8:25:G:O4' | 2.05 | 0.56 |
| 11:HH:28:THR:HG22 | 11:HH:33:VAL:HG12 | 1.88 | 0.56 |
| 62:O:129:LYS:HA | 81:2:989:C:H4' | 1.88 | 0.56 |
| 83:1:405:VAL:HA | 83:1:406:LYS:CB | 2.35 | 0.55 |
| 1:5:1196:A:N7 | 1:5:1197:G:C6 | 2.74 | 0.55 |
| 1:5:2239:A:C6 | 1:5:2240:A:N6 | 2.74 | 0.55 |
| 1:5:3182:U:C5 | 15:MM:121:LEU:HD22 | 2.41 | 0.55 |
| 56:I:103:GLN:HA | 56:I:166:LEU:O | 2.06 | 0.55 |
| 17:OO:192[A]:GLU:O | 17:OO:194[A]:LEU:CA | 2.53 | 0.55 |
| 82:4:6120:U:HO2' | 82:4:6121:A:P | 2.28 | 0.55 |
| 1:5:173:G:C6 | 1:5:174:C:C4 | 2.94 | 0.55 |
| 1:5:2218:G:HO2' | 1:5:2219:G:P | 2.27 | 0.55 |
| 1:5:522:A:H2' | 1:5:523:G:C8 | 2.41 | 0.55 |
| 2:7:73:C:O4' | 2:7:73:C:O2 | 2.24 | 0.55 |
| 28:ZZ:46:ILE:HD11 | 28:ZZ:49:TYR:CE2 | 2.42 | 0.55 |
| 83:1:684:VAL:HG21 | 83:1:717:PHE:CZ | 2.41 | 0.55 |
| 81:2:886:A:N7 | 81:2:887:U:C4 | 2.74 | 0.55 |
| 81:2:886:A:N1 | 81:2:925:A:C2 | 2.73 | 0.55 |
| 1:5:1106:A:C2 | 1:5:1107:A:C8 | 2.94 | 0.55 |
| 1:5:2506:U:O2 | 1:5:2506:U:H2' | 2.06 | 0.55 |
| 1:5:3224:G:C6 | 1:5:3225:C:C4 | 2.94 | 0.55 |
| 27:YY:102:SER:OG | 27:YY:103:LYS:NZ | 2.39 | 0.55 |
| 81:2:100:A:H2' | 81:2:101:U:O4' | 2.07 | 0.55 |
| 81:2:1540:G:C6 | 81:2:1566:C:N3 | 2.74 | 0.55 |
| 59:L:103:ARG:NH1 | 81:2:306:G:OP1 | 2.39 | 0.55 |
| 1:5:1197:G:C6 | 1:5:1198:C:N4 | 2.74 | 0.55 |
| 1:5:1459:G:C2 | 1:5:1460:A:C8 | 2.94 | 0.55 |
| 1:5:792:U:O2' | 1:5:883:G:OP1 | 2.21 | 0.55 |
| 7:DD:61:ILE:HG23 | 7:DD:79:TYR:CE2 | 2.42 | 0.55 |
| 17:OO:172[A]:LYS:O | 17:OO:173[A]:LYS:O | 2.24 | 0.55 |
| 83:1:645:LEU:O | 83:1:684:VAL:O | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 83:1:750:LYS:C | 83:1:751:ARG:HG3 | 2.25 | 0.55 |
| 81:2:930:C:H3' | 81:2:931:U:C5' | 2.37 | 0.55 |
| 1:5:1791:C:HO2' | 1:5:1792:A:H8 | 1.51 | 0.55 |
| 1:5:2277:C:C5' | 1:5:2278:A:H5' | 2.36 | 0.55 |
| 54:G:154:ARG:HB3 | 81:2:77:U:H4' | 1.88 | 0.55 |
| 14:LL:2:ALA:O | 14:LL:3:ILE:CB | 2.51 | 0.55 |
| 70:W:82:LYS:O | 70:W:84:ALA:N | 2.39 | 0.55 |
| 83:1:579:SER:CB | 83:1:580:PRO:CD | 2.84 | 0.55 |
| 54:G:154:ARG:CB | 81:2:77:U:H4' | 2.37 | 0.55 |
| 1:5:2749:U:H2' | 1:5:2750:U:C6 | 2.41 | 0.55 |
| 19:QQ:124:LEU:N | 82:4:6039:A:C4 | 120.46 | 0.55 |
| 83:1:464:LEU:O | 83:1:466:THR:N | 2.35 | 0.55 |
| 83:1:579:SER:OG | 83:1:704:GLN:O | 2.14 | 0.55 |
| 83:1:72:SER:HB3 | 83:1:73:THR:HA | 1.89 | 0.55 |
| 1:5:2277:C:H4' | 1:5:2278:A:H4' | 1.89 | 0.55 |
| 1:5:2543:G:C2 | 1:5:2544:G:C8 | 2.94 | 0.55 |
| 17:OO:126[A]:ARG:HD3 | 17:OO:136[A]:TYR:CE2 | 2.41 | 0.55 |
| 17:OO:166[A]:ALA:O | 17:OO:169[A]:TYR:N | 2.36 | 0.55 |
| 68:U:34:LEU:HD11 | 68:U:89:ARG:HG3 | 1.87 | 0.55 |
| 83:1:684:VAL:HG21 | 83:1:717:PHE:CE1 | 2.42 | 0.55 |
| 1:5:1927:G:C6 | 1:5:2055:G:O4' | 2.59 | 0.55 |
| 1:5:2214:C:H2' | 1:5:2215:G:O4' | 2.07 | 0.55 |
| 1:5:2480:A:OP2 | 1:5:2481:C:H5'' | 2.05 | 0.55 |
| 1:5:593:U:O2' | 1:5:594:A:OP1 | 2.22 | 0.55 |
| 17:OO:182[A]:LYS:O | 17:OO:185[A]:THR:HG22 | 2.06 | 0.55 |
| 81:2:116:U:O2' | 81:2:332:A:N3 | 2.29 | 0.55 |
| 1:5:1337:A:OP1 | 1:5:1338:G:OP2 | 2.25 | 0.55 |
| 1:5:541:G:H2' | 1:5:542:A:O4' | 2.07 | 0.55 |
| 6:CC:342:LYS:O | 6:CC:343:LYS:C | 2.46 | 0.55 |
| 52:E:67:GLN:HA | 52:E:68:ARG:HB2 | 1.87 | 0.55 |
| 17:OO:117[A]:LYS:HG3 | 17:OO:118[A]:ARG:O | 2.06 | 0.55 |
| 17:OO:119[A]:VAL:O | 17:OO:119[A]:VAL:HG22 | 2.06 | 0.55 |
| 83:1:701:GLY:HA2 | 83:1:702:GLY:C | 2.28 | 0.55 |
| 81:2:923:A:O2' | 81:2:985:G:O3' | 2.25 | 0.55 |
| 1:5:1587:G:N2 | 1:5:1796:C:C2 | 2.75 | 0.55 |
| 1:5:436:A:N6 | 1:5:594:A:C8 | 2.74 | 0.55 |
| 1:5:869:U:H2' | 1:5:870:U:O4' | 2.07 | 0.55 |
| 52:E:128:LYS:O | 52:E:140:VAL:N | 2.36 | 0.55 |
| 14:LL:27:ASP:O | 14:LL:30:GLY:N | 2.39 | 0.55 |
| 17:OO:66[A]:ASN:C | 17:OO:68[A]:THR:N | 2.60 | 0.55 |
| 1:5:2358:C:OP1 | 18:PP:66:SER:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 81:2:111:U:H2' | 81:2:112:A:O4' | 2.07 | 0.54 |
| 81:2:1527:C:H2' | 81:2:1528:C:C6 | 2.43 | 0.54 |
| 81:2:309:C:C2 | 81:2:356:G:C2 | 2.94 | 0.54 |
| 1:5:1464:G:N2 | 1:5:1464:G:OP2 | 2.38 | 0.54 |
| 17:OO:139[A]:LEU:O | 17:OO:140[A]:GLY:C | 2.45 | 0.54 |
| 1:5:216:G:OP1 | 27:YY:16:ARG:NH1 | 2.40 | 0.54 |
| 82:4:6117:C:H2' | 82:4:6118:U:O4' | 2.07 | 0.54 |
| 1:5:3245:U:O2 | 1:5:3245:U:O4' | 2.25 | 0.54 |
| 1:5:2996:G:OP1 | 83:1:27:HIS:CE1 | 2.60 | 0.54 |
| 81:2:1012:A:H2' | 81:2:1013:G:O4' | 2.07 | 0.54 |
| 81:2:152:G:H2' | 81:2:153:G:C8 | 2.43 | 0.54 |
| 54:G:154:ARG:C | 81:2:78:A:O5' | 2.45 | 0.54 |
| 1:5:83:U:H2' | 1:5:84:U:O4' | 2.06 | 0.54 |
| 10:GG:133:TYR:CG | 10:GG:189:VAL:HG21 | 2.43 | 0.54 |
| 17:OO:150[A]:TYR:N | 17:OO:150[A]:TYR:CD1 | 2.76 | 0.54 |
| 81:2:874:G:H2' | 81:2:876:G:OP2 | 2.07 | 0.54 |
| 1:5:1346:G:N2 | 1:5:1347:C:C2 | 2.76 | 0.54 |
| 1:5:1356:C:OP1 | 6:CC:141:ARG:NH1 | 2.39 | 0.54 |
| 1:5:1370:A:C2 | 3:8:8:C:H5' | 2.42 | 0.54 |
| 1:5:1925:G:C2' | 1:5:2056:C:O2 | 2.55 | 0.54 |
| 1:5:2237:U:N3 | 1:5:2241:G:N1 | 2.54 | 0.54 |
| 55:H:135:ILE:HG23 | 55:H:152:ILE:HG23 | 1.88 | 0.54 |
| 22:TT:11:THR:O | 22:TT:12:ARG:C | 2.45 | 0.54 |
| 83:1:107:GLY:HA2 | 83:1:138:GLN:HE22 | 1.72 | 0.54 |
| 82:4:6173:C:C2' | 82:4:6173:C:O2 | 2.56 | 0.54 |
| 1:5:1209:C:O2' | 1:5:1210:C:OP1 | 2.17 | 0.54 |
| 1:5:1862:A:C6 | 1:5:1863:U:C4 | 2.95 | 0.54 |
| 1:5:2480:A:H4' | 10:GG:248:ARG:NH2 | 2.22 | 0.54 |
| 1:5:2971:G:N1 | 1:5:2972:C:C4 | 2.76 | 0.54 |
| 1:5:303:G:C2 | 1:5:313:A:C2 | 2.96 | 0.54 |
| 1:5:312:C:C2 | 1:5:2746:G:C2 | 2.95 | 0.54 |
| 6:CC:31:ARG:HB2 | 6:CC:34:ILE:HG22 | 1.89 | 0.54 |
| 56:I:139:ASN:HB2 | 81:2:186:G:H2' | 1.90 | 0.54 |
| 70:W:2:THR:N | 81:2:1033:C:HO2' | 2.04 | 0.54 |
| 72:Y:29:HIS:CD2 | 72:Y:35:VAL:HG13 | 2.43 | 0.54 |
| 83:1:462:PHE:O | 83:1:463:LEU:HD22 | 2.07 | 0.54 |
| 83:1:701:GLY:CA | 83:1:703:GLY:N | 2.71 | 0.54 |
| 81:2:1586:G:C6 | 81:2:1587:C:C4 | 2.95 | 0.54 |
| 81:2:991:A:N1 | 81:2:1011:U:C4 | 2.75 | 0.54 |
| 1:5:3085:C:H2' | 1:5:3086:C:O4' | 2.08 | 0.54 |
| 1:5:3224:G:N1 | 1:5:3225:C:C2 | 2.76 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5:314:U:OP1 | 14:LL:104:ARG:NH2 | 2.41 | 0.54 |
| 81:2:1439:C:H2' | 81:2:1440:U:C5' | 2.38 | 0.54 |
| 81:2:1643:G:N2 | 81:2:1644:C:C2 | 2.75 | 0.54 |
| 81:2:1671:G:C2 | 81:2:1672:C:C2 | 2.96 | 0.54 |
| 81:2:884:G:C3' | 81:2:885:U:C4' | 2.86 | 0.54 |
| 1:5:1562:A:H2' | 1:5:1563:A:C8 | 2.42 | 0.54 |
| 1:5:2277:C:H5' | 1:5:2278:A:H5' | 1.88 | 0.54 |
| 17:OO:138[A]:THR:O | 17:OO:140[A]:GLY:N | 2.40 | 0.54 |
| 22:TT:11:THR:O | 22:TT:14:MET:N | 2.38 | 0.54 |
| 83:1:693:LEU:HB3 | 83:1:700:ARG:NH1 | 2.22 | 0.54 |
| 81:2:970:A:C8 | 81:2:971:G:C8 | 2.95 | 0.54 |
| 82:4:6044:G:N2 | 82:4:6045:C:C2 | 2.76 | 0.54 |
| 1:5:634:G:N1 | 1:5:773:C:C2 | 2.76 | 0.54 |
| 6:CC:93:MET:HG2 | 6:CC:94:CYS:SG | 2.48 | 0.54 |
| 14:LL:5:LYS:N | 14:LL:5:LYS:HD2 | 2.03 | 0.54 |
| 8:EE:157:TYR:CE1 | 15:MM:115:PHE:HA | 2.42 | 0.54 |
| 17:OO:58[A]:TYR:C | 17:OO:60[A]:ARG:H | 2.11 | 0.54 |
| 1:5:643:C:OP1 | 19:QQ:147:ARG:NH2 | 2.40 | 0.54 |
| 83:1:587:TYR:CE2 | 83:1:690:ASP:CB | 2.90 | 0.54 |
| 83:1:587:TYR:O | 83:1:588:LEU:HG | 2.08 | 0.54 |
| 81:2:427:A:C2 | 81:2:439:U:O2 | 2.61 | 0.54 |
| 82:4:6127:C:N3 | 82:4:6160:G:C6 | 2.76 | 0.54 |
| 1:5:1491:G:H2' | 1:5:1492:G:O4' | 2.07 | 0.54 |
| 1:5:2480:A:C2' | 1:5:2481:C:H4' | 2.37 | 0.54 |
| 1:5:2500:C:O2 | 1:5:2500:C:O4' | 2.26 | 0.54 |
| 1:5:3255:C:H2' | 1:5:3256:A:H5' | 1.90 | 0.54 |
| 3:8:7:U:O4 | 3:8:8:C:N4 | 2.41 | 0.54 |
| 9:FF:160:LEU:HD22 | 9:FF:166:VAL:HG22 | 1.89 | 0.54 |
| 14:LL:5:LYS:O | 14:LL:7:LEU:CB | 2.53 | 0.54 |
| 17:OO:159[A]:GLU:O | 17:OO:161[A]:ARG:N | 2.41 | 0.54 |
| 17:OO:17[A]:LEU:C | 17:OO:19[A]:ARG:N | 2.59 | 0.54 |
| 83:1:694:HIS:N | 83:1:694:HIS:CD2 | 2.75 | 0.54 |
| 81:2:887:U:O4 | 81:2:888:U:O4 | 2.26 | 0.54 |
| 62:O:41:ARG:NH2 | 81:2:915:U:O2 | 2.41 | 0.54 |
| 1:5:3252:G:C2 | 1:5:3253:C:C2 | 2.95 | 0.54 |
| 7:DD:104:LEU:HD21 | 7:DD:108:ARG:CZ | 2.37 | 0.54 |
| 83:1:682:ARG:NE | 83:1:801:TRP:CE3 | 2.76 | 0.53 |
| 81:2:9:U:O2 | 81:2:12:U:H5 | 1.91 | 0.53 |
| 81:2:480:A:N1 | 81:2:506:U:C5 | 2.73 | 0.53 |
| 81:2:975:G:H1 | 81:2:1022:A:HO2' | 1.55 | 0.53 |
| 1:5:3138:A:H2' | 1:5:3139:U:H5' | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 83:1:519:LEU:HG | 83:1:531:ALA:HB2 | 1.90 | 0.53 |
| 83:1:560:VAL:HB | 83:1:561:VAL:HA | 1.89 | 0.53 |
| 83:1:583:HIS:CE1 | 83:1:704:GLN:CG | 2.89 | 0.53 |
| 51:D:176:LEU:HB3 | 51:D:177:LEU:HA | 1.89 | 0.53 |
| 17:OO:148[A]:TRP:CE3 | 17:OO:150[A]:TYR:O | 2.61 | 0.53 |
| 17:OO:161[A]:ARG:CG | 17:OO:162[A]:LYS:N | 2.64 | 0.53 |
| 17:OO:55[A]:TYR:OH | 17:OO:74[A]:PHE:O | 2.26 | 0.53 |
| 24:VV:20:GLY:O | 24:VV:21:ALA:C | 2.46 | 0.53 |
| 1:5:185:C:O2 | 1:5:232:G:C2 | 2.61 | 0.53 |
| 1:5:2218:G:O5' | 1:5:2242:G:C8 | 2.61 | 0.53 |
| 4:AA:223:SER:O | 4:AA:237:LEU:N | 2.40 | 0.53 |
| 5:BB:53:MET:HG2 | 5:BB:77:THR:HG22 | 1.89 | 0.53 |
| 9:FF:128:GLU:HG2 | 9:FF:129:PRO:HD3 | 1.91 | 0.53 |
| 81:2:1671:G:C5 | 81:2:1672:C:N4 | 2.76 | 0.53 |
| 1:5:1210:C:O2 | 1:5:1221:G:C2 | 2.61 | 0.53 |
| 1:5:1361:A:N3 | 1:5:1361:A:H5' | 2.22 | 0.53 |
| 1:5:2167:A:H2' | 1:5:2168:G:C5' | 2.38 | 0.53 |
| 1:5:2218:G:C5' | 1:5:2242:G:C8 | 2.92 | 0.53 |
| 1:5:3131:G:C6 | 1:5:3256:A:C6 | 2.97 | 0.53 |
| 17:OO:19[A]:ARG:O | 17:OO:22[A]:SER:N | 2.36 | 0.53 |
| 83:1:204:PRO:HA | 83:1:209:VAL:HG11 | 1.89 | 0.53 |
| 83:1:584:ASN:OD1 | 83:1:585:ARG:N | 2.42 | 0.53 |
| 81:2:700:C:C2 | 81:2:739:G:N1 | 2.77 | 0.53 |
| 1:5:1882:A:N3 | 1:5:2089:A:H2' | 2.23 | 0.53 |
| 1:5:2248:A:C2 | 1:5:2257:G:C6 | 2.97 | 0.53 |
| 1:5:602:A:C2 | 1:5:603:A:C4 | 2.97 | 0.53 |
| 1:5:77:A:H2' | 1:5:78:U:O4' | 2.09 | 0.53 |
| 2:7:25:G:H2' | 2:7:26:C:O4' | 2.08 | 0.53 |
| 4:AA:9:ARG:O | 4:AA:12:ALA:N | 2.42 | 0.53 |
| 17:OO:194[A]:LEU:O | 17:OO:195[A]:ALA:C | 2.44 | 0.53 |
| 81:2:1002:A:O2' | 81:2:1004:A:N7 | 2.32 | 0.53 |
| 81:2:1108:G:C5 | 81:2:1109:G:N7 | 2.76 | 0.53 |
| 81:2:1173:C:N4 | 81:2:1464:G:C6 | 2.77 | 0.53 |
| 81:2:1770:C:H6 | 81:2:1770:C:H5'' | 1.73 | 0.53 |
| 1:5:413:U:O2 | 1:5:414:U:C2 | 2.61 | 0.53 |
| 1:5:436:A:C6 | 1:5:597:G:N1 | 2.77 | 0.53 |
| 1:5:634:G:O6 | 1:5:773:C:C4 | 2.62 | 0.53 |
| 3:8:8:C:O2' | 3:8:9:A:O5' | 2.21 | 0.53 |
| 17:OO:12[A]:GLY:O | 17:OO:13[A]:LYS:O | 2.26 | 0.53 |
| 17:OO:148[A]:TRP:CD2 | 17:OO:150[A]:TYR:O | 2.61 | 0.53 |
| 81:2:1440:U:O2' | 81:2:1441:U:H5' | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 81:2:1673:C:C2 | 81:2:1725:G:N2 | 2.77 | 0.53 |
| 1:5:1119:G:N2 | 1:5:1127:C:C2 | 2.76 | 0.53 |
| 1:5:1119:G:C2 | 1:5:1127:C:C2 | 2.97 | 0.53 |
| 1:5:1372:G:N2 | 1:5:1373:C:C2 | 2.77 | 0.53 |
| 1:5:2216:G:N3 | 1:5:2240:A:C2 | 2.77 | 0.53 |
| 83:1:108:HIS:O | 83:1:110:ASP:N | 2.41 | 0.53 |
| 83:1:481:MET:HA | 83:1:482:LYS:CB | 2.39 | 0.53 |
| 71:X:89:ASN:N | 81:2:568:C:OP1 | 2.39 | 0.53 |
| 82:4:6194:C:O2' | 82:4:6195:G:O4' | 2.27 | 0.53 |
| 1:5:22:G:H1' | 3:8:104:A:N3 | 2.24 | 0.53 |
| 1:5:703:C:C2 | 1:5:711:G:C2 | 2.97 | 0.53 |
| 12:II:23:ASN:O | 12:II:25:ALA:N | 2.42 | 0.53 |
| 16:NN:156:HIS:HB3 | 16:NN:159:ARG:HD2 | 1.90 | 0.53 |
| 1:5:1916:G:H5'' | 20:RR:134:HIS:CE1 | 2.44 | 0.53 |
| 28:ZZ:40:HIS:CD2 | 28:ZZ:74:VAL:HG13 | 2.44 | 0.53 |
| 83:1:388:THR:HG23 | 83:1:394:PHE:HA | 1.91 | 0.53 |
| 83:1:52:GLY:N | 83:1:53:GLU:HB2 | 2.24 | 0.53 |
| 83:1:684:VAL:HG12 | 83:1:686:VAL:CB | 2.26 | 0.53 |
| 1:5:114:A:C2' | 1:5:115:A:H5' | 2.39 | 0.53 |
| 1:5:1773:A:H2' | 1:5:1774:C:C6 | 2.44 | 0.53 |
| 1:5:2061:A:H1' | 1:5:2062:A:C8 | 2.44 | 0.53 |
| 1:5:2224:A:C6 | 1:5:2229:U:O2 | 2.61 | 0.53 |
| 1:5:2406:G:C2 | 1:5:2479:U:C2 | 2.97 | 0.53 |
| 1:5:2864:A:H5'' | 1:5:2864:A:H8 | 1.73 | 0.53 |
| 17:OO:98[A]:ALA:O | 17:OO:99[A]:ALA:O | 2.25 | 0.53 |
| 24:VV:17:LEU:HD11 | 24:VV:98:ASN:CB | 2.39 | 0.53 |
| 83:1:572:SER:HA | 83:1:589:LYS:HG3 | 1.91 | 0.53 |
| 83:1:582:LYS:HZ1 | 83:1:694:HIS:CG | 2.27 | 0.53 |
| 83:1:705:ILE:CA | 83:1:708:THR:CG2 | 2.61 | 0.53 |
| 81:2:542:C:O2 | 81:2:542:C:O4' | 2.25 | 0.53 |
| 1:5:1197:G:C2 | 1:5:1198:C:C2 | 2.97 | 0.53 |
| 1:5:1928:A:N6 | 1:5:2053:C:C4 | 2.77 | 0.53 |
| 1:5:2218:G:C4 | 1:5:2219:G:C1' | 2.92 | 0.53 |
| 1:5:2480:A:C6 | 1:5:2481:C:C2 | 2.97 | 0.53 |
| 1:5:2510:U:H2' | 1:5:2510:U:O2 | 2.08 | 0.53 |
| 1:5:2635:A:N6 | 1:5:2655:G:O2' | 2.42 | 0.53 |
| 1:5:3243:U:HO2' | 1:5:3244:G:C4' | 2.22 | 0.53 |
| 1:5:340:C:N4 | 1:5:341:G:C6 | 2.77 | 0.53 |
| 10:GG:150:VAL:HG23 | 10:GG:174:VAL:HG11 | 1.91 | 0.53 |
| 17:OO:24[A]:VAL:HG13 | 17:OO:24[A]:VAL:O | 2.08 | 0.53 |
| 82:4:6200:A:H4' | 82:4:6201:C:O5' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:5:1052:U:O4' | 1:5:1052:U:O2 | 2.27 | 0.52 |
| 1:5:412:G:C5 | 1:5:413:U:C5 | 2.97 | 0.52 |
| 1:5:503:A:C6 | 1:5:504:A:N6 | 2.77 | 0.52 |
| 1:5:650:A:N1 | 1:5:676:G:O2' | 2.38 | 0.52 |
| 12:II:49:CYS:HG | 12:II:51:HIS:CE1 | 2.27 | 0.52 |
| 57:J:12:TYR:CG | 57:J:44:ARG:HA | 2.44 | 0.52 |
| 13:JJ:102:PHE:CE2 | 13:JJ:129:ILE:HD13 | 2.45 | 0.52 |
| 17:OO:186[A]:VAL:O | 17:OO:187[A]:GLY:O | 2.25 | 0.52 |
| 81:2:1438:C:O2 | 81:2:1438:C:H2' | 2.08 | 0.52 |
| 81:2:1440:U:O5' | 81:2:1440:U:H6 | 1.93 | 0.52 |
| 1:5:1284:G:O2' | 1:5:1289:A:N1 | 2.31 | 0.52 |
| 1:5:2029:G:C2 | 1:5:2030:C:C2 | 2.97 | 0.52 |
| 1:5:2251:U:O2 | 1:5:2279:U:H4' | 2.09 | 0.52 |
| 1:5:2304:G:N2 | 1:5:2308:C:O2' | 2.42 | 0.52 |
| 1:5:628:C:H2' | 1:5:629:A:C8 | 2.44 | 0.52 |
| 1:5:659:G:C2 | 1:5:668:C:C2 | 2.97 | 0.52 |
| 3:8:15:G:C6 | 3:8:16:G:N1 | 2.77 | 0.52 |
| 54:G:155:ASP:O | 54:G:157:VAL:HB | 2.09 | 0.52 |
| 11:HH:112:ILE:HD13 | 11:HH:161:ILE:HD11 | 1.90 | 0.52 |
| 17:OO:156[A]:LYS:O | 17:OO:157[A]:LEU:C | 2.48 | 0.52 |
| 17:OO:39[A]:ALA:O | 17:OO:42[A]:LEU:N | 2.38 | 0.52 |
| 83:1:823:ARG:NH1 | 83:1:829:LYS:O | 2.42 | 0.52 |
| 81:2:1363:G:N1 | 81:2:1364:C:C4 | 2.78 | 0.52 |
| 1:5:1159:U:H3 | 1:5:1288:A:N6 | 2.08 | 0.52 |
| 1:5:12:A:H2' | 1:5:13:A:C8 | 2.45 | 0.52 |
| 1:5:2438:G:C2 | 1:5:2439:C:C4 | 2.98 | 0.52 |
| 1:5:436:A:C6 | 1:5:596:U:O4 | 2.61 | 0.52 |
| 1:5:1019:A:H2' | 12:II:22:TYR:CZ | 2.45 | 0.52 |
| 19:QQ:32:LEU:C | 19:QQ:32:LEU:HD23 | 2.29 | 0.52 |
| 1:5:1291:C:O2 | 21:SS:115:ARG:NH2 | 2.43 | 0.52 |
| 83:1:576:LEU:HB3 | 83:1:585:ARG:NH2 | 2.25 | 0.52 |
| 81:2:1786:G:H2' | 81:2:1787:G:O4' | 2.10 | 0.52 |
| 81:2:360:C:C2 | 81:2:383:G:N2 | 2.77 | 0.52 |
| 1:5:1791:C:O2' | 1:5:1792:A:C8 | 2.62 | 0.52 |
| 1:5:287:G:C2 | 1:5:288:C:C2 | 2.97 | 0.52 |
| 1:5:532:A:N6 | 1:5:533:G:C2 | 2.78 | 0.52 |
| 17:OO:126[A]:ARG:HG2 | 17:OO:126[A]:ARG:O | 2.10 | 0.52 |
| 17:OO:14[A]:GLY:O | 17:OO:15[A]:HIS:C | 2.47 | 0.52 |
| 17:OO:163[A]:ALA:O | 17:OO:166[A]:ALA:HB3 | 2.09 | 0.52 |
| 83:1:441:PHE:HB2 | 83:1:442:VAL:HB | 1.92 | 0.52 |
| 83:1:828:MET:HB3 | 83:1:829:LYS:HA | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 81:2:425:G:N2 | 81:2:426:C:C2 | 2.77 | 0.52 |
| 81:2:700:C:N3 | 81:2:739:G:C6 | 2.78 | 0.52 |
| 81:2:883:A:O2' | 81:2:884:G:H5' | 2.09 | 0.52 |
| 82:4:6198:A:C2 | 82:4:6199:A:C6 | 2.98 | 0.52 |
| 1:5:1584:C:H2' | 1:5:1585:U:C6 | 2.45 | 0.52 |
| 1:5:2201:A:H2' | 1:5:2202:A:O4' | 2.10 | 0.52 |
| 1:5:2277:C:H4' | 1:5:2278:A:C4' | 2.40 | 0.52 |
| 1:5:2482:U:O2' | 1:5:2483:U:H2' | 2.10 | 0.52 |
| 1:5:2482:U:O4 | 1:5:2560:G:C4 | 2.62 | 0.52 |
| 1:5:518:C:O2 | 1:5:518:C:C2' | 2.57 | 0.52 |
| 3:8:6:U:O2' | 3:8:7:U:H5' | 2.10 | 0.52 |
| 6:CC:74:ILE:HG21 | 6:CC:88:ALA:HB1 | 1.91 | 0.52 |
| 17:OO:114[A]:ASP:OD1 | 17:OO:114[A]:ASP:N | 2.41 | 0.52 |
| 17:OO:168[A]:TYR:CE1 | 17:OO:168[A]:TYR:O | 2.54 | 0.52 |
| 17:OO:17[A]:LEU:C | 17:OO:19[A]:ARG:H | 2.12 | 0.52 |
| 83:1:77:LEU:HB3 | 83:1:78:TYR:HB2 | 1.91 | 0.52 |
| 1:5:1926:U:C4 | 1:5:1927:G:N7 | 2.77 | 0.52 |
| 1:5:2234:C:C2' | 1:5:2235:U:C5' | 2.70 | 0.52 |
| 1:5:513:U:H2' | 1:5:514:G:H1' | 1.92 | 0.52 |
| 1:5:957:U:C2 | 1:5:958:U:C6 | 2.98 | 0.52 |
| 4:AA:101:VAL:HG22 | 4:AA:165:VAL:HG22 | 1.91 | 0.52 |
| 12:II:31:ILE:O | 12:II:31:ILE:HG23 | 2.09 | 0.52 |
| 17:OO:15[A]:HIS:NE2 | 17:OO:121[A]:VAL:N | 2.58 | 0.52 |
| 24:VV:84:ALA:HA | 24:VV:94:TYR:HB3 | 1.92 | 0.52 |
| 83:1:69:THR:N | 86:1:902:GCP:O3G | 2.42 | 0.52 |
| 81:2:1752:A:H3' | 81:2:1754:A:C2 | 2.44 | 0.52 |
| 81:2:776:G:N2 | 81:2:777:C:C2 | 2.78 | 0.52 |
| 1:5:128:G:C2 | 1:5:141:C:O2 | 2.63 | 0.52 |
| 1:5:2238:U:C5 | 1:5:2239:A:C5 | 2.95 | 0.52 |
| 1:5:2480:A:C5 | 1:5:2481:C:C2 | 2.98 | 0.52 |
| 1:5:504:A:H2 | 1:5:532:A:N1 | 2.08 | 0.52 |
| 1:5:646:U:H2' | 1:5:647:G:H8 | 1.74 | 0.52 |
| 17:OO:52[A]:LYS:CG | 17:OO:52[A]:LYS:O | 2.58 | 0.52 |
| 83:1:582:LYS:NZ | 83:1:694:HIS:CG | 2.78 | 0.52 |
| 83:1:695:ALA:CA | 83:1:700:ARG:HH12 | 2.19 | 0.52 |
| 81:2:886:A:H2' | 81:2:887:U:O4' | 2.10 | 0.52 |
| 81:2:888:U:C1' | 81:2:987:A:H4' | 2.40 | 0.52 |
| 1:5:13:A:C6 | 1:5:15:C:C4 | 2.98 | 0.52 |
| 1:5:1665:A:H2' | 1:5:1666:A:C8 | 2.45 | 0.52 |
| 1:5:1833:A:OP1 | 20:RR:83:GLY:N | 2.39 | 0.52 |
| 1:5:2218:G:N9 | 1:5:2219:G:O4' | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:5:294:U:P | 16:NN:15:GLN:HE22 | 2.33 | 0.52 |
| 17:OO:48[A]:PHE:CD1 | 17:OO:48[A]:PHE:C | 2.82 | 0.52 |
| 17:OO:8[A]:VAL:O | 17:OO:35[A]:VAL:HG12 | 2.08 | 0.52 |
| 83:1:579:SER:HB3 | 83:1:580:PRO:CD | 2.40 | 0.52 |
| 83:1:579:SER:CB | 83:1:580:PRO:HD3 | 2.39 | 0.52 |
| 81:2:1007:G:H2' | 81:2:1008:U:C6 | 2.45 | 0.52 |
| 81:2:1771:C:C2 | 81:2:1787:G:C2 | 2.98 | 0.52 |
| 1:5:2222:G:C6 | 1:5:2223:U:C5 | 2.97 | 0.52 |
| 1:5:2804:C:O2 | 1:5:2804:C:O4' | 2.28 | 0.52 |
| 4:AA:80:GLU:HG3 | 4:AA:170:ALA:HA | 1.92 | 0.52 |
| 5:BB:305:ILE:HD12 | 5:BB:321:PHE:CZ | 2.44 | 0.52 |
| 17:OO:50[A]:ARG:HG2 | 17:OO:50[A]:ARG:NH1 | 2.22 | 0.52 |
| 17:OO:60[A]:ARG:HG3 | 17:OO:60[A]:ARG:O | 2.07 | 0.52 |
| 1:5:1601:A:N7 | 1:5:1613:C:H2' | 2.25 | 0.52 |
| 1:5:2029:G:C6 | 1:5:2030:C:C4 | 2.98 | 0.52 |
| 1:5:2361:C:O2 | 1:5:2955:A:N1 | 2.42 | 0.52 |
| 1:5:3056:G:C2 | 1:5:3057:C:C2 | 2.98 | 0.52 |
| 1:5:960:A:H2' | 1:5:961:U:O4' | 2.09 | 0.52 |
| 3:8:7:U:C4 | 3:8:8:C:N4 | 2.78 | 0.52 |
| 6:CC:349:ILE:HD12 | 6:CC:350:LYS:HA | 1.92 | 0.52 |
| 17:OO:171[A]:LYS:HZ2 | 17:OO:171[A]:LYS:HB3 | 1.73 | 0.52 |
| 83:1:694:HIS:N | 83:1:695:ALA:CA | 2.73 | 0.51 |
| 81:2:25:C:O4' | 81:2:25:C:O2 | 2.25 | 0.51 |
| 81:2:287:A:H2' | 81:2:288:U:O4' | 2.10 | 0.51 |
| 1:5:1923:G:C2 | 1:5:1925:G:H8 | 2.08 | 0.51 |
| 1:5:2055:G:C6 | 1:5:2056:C:N4 | 2.55 | 0.51 |
| 1:5:2060:U:O4' | 1:5:2060:U:O2 | 2.27 | 0.51 |
| 1:5:2662:A:C2 | 1:5:2663:A:C2 | 2.98 | 0.51 |
| 5:BB:119:TYR:OH | 5:BB:129:ALA:N | 2.43 | 0.51 |
| 17:OO:158[A]:GLU:O | 17:OO:160[A]:LYS:N | 2.42 | 0.51 |
| 18:PP:148:LEU:HD12 | 18:PP:148:LEU:C | 2.31 | 0.51 |
| 81:2:992:A:N6 | 81:2:993:G:C4 | 2.78 | 0.51 |
| 1:5:2219:G:O5' | 1:5:2277:C:C6 | 2.63 | 0.51 |
| 1:5:3303:A:N7 | 1:5:3338:A:O2' | 2.35 | 0.51 |
| 1:5:529:U:C2 | 1:5:532:A:C5 | 2.97 | 0.51 |
| 3:8:118:C:C2 | 3:8:136:G:C2 | 2.97 | 0.51 |
| 4:AA:192:LYS:HB3 | 4:AA:193:ARG:HG2 | 1.92 | 0.51 |
| 5:BB:11:HIS:ND1 | 5:BB:234:GLY:O | 2.43 | 0.51 |
| 57:J:149:ARG:O | 57:J:151:GLU:N | 2.42 | 0.51 |
| 17:OO:15[A]:HIS:HB3 | 17:OO:20[A]:LEU:HB2 | 1.93 | 0.51 |
| 17:OO:54[A]:LYS:O | 17:OO:57[A]:ASP:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 71:X:102:VAL:HG22 | 71:X:124:VAL:HG13 | 1.92 | 0.51 |
| 71:X:63:GLN:HB3 | 71:X:64:PRO:CD | 2.41 | 0.51 |
| 83:1:701:GLY:HA3 | 83:1:704:GLN:N | 2.26 | 0.51 |
| 81:2:929:A:HO2' | 81:2:930:C:P | 2.33 | 0.51 |
| 1:5:1417:A:N1 | 1:5:2325:A:H5'' | 2.26 | 0.51 |
| 1:5:1601:A:OP1 | 28:ZZ:69:LYS:NZ | 2.44 | 0.51 |
| 1:5:2313:U:H2' | 1:5:2314:A:H8 | 1.73 | 0.51 |
| 1:5:2480:A:P | 1:5:2481:C:C5' | 2.91 | 0.51 |
| 1:5:967:A:H2' | 1:5:968:A:O4' | 2.10 | 0.51 |
| 7:DD:166:ALA:HB1 | 7:DD:171:LEU:HD12 | 1.92 | 0.51 |
| 57:J:79:ARG:NH2 | 81:2:763:G:OP2 | 2.42 | 0.51 |
| 14:LL:54:LEU:HD13 | 14:LL:75:PHE:CE2 | 2.45 | 0.51 |
| 18:PP:52:LEU:HD13 | 18:PP:88:VAL:HG11 | 1.92 | 0.51 |
| 83:1:577:SER:CB | 83:1:586:ILE:H | 2.23 | 0.51 |
| 81:2:1138:A:H2' | 81:2:1139:G:O4' | 2.10 | 0.51 |
| 81:2:1440:U:C5' | 81:2:1445:C:N4 | 2.73 | 0.51 |
| 81:2:1464:G:N1 | 81:2:1465:C:C4 | 2.78 | 0.51 |
| 1:5:1924:C:N3 | 1:5:2055:G:C6 | 2.73 | 0.51 |
| 1:5:2200:C:O2 | 1:5:2200:C:O4' | 2.25 | 0.51 |
| 1:5:2224:A:C2 | 1:5:2225:A:N6 | 2.78 | 0.51 |
| 1:5:502:G:N2 | 1:5:535:C:C2 | 2.79 | 0.51 |
| 81:2:1072:G:C2 | 81:2:1073:G:C8 | 2.99 | 0.51 |
| 81:2:1670:G:H2' | 81:2:1671:G:C8 | 2.45 | 0.51 |
| 81:2:1794:C:O4' | 81:2:1794:C:O2 | 2.28 | 0.51 |
| 81:2:585:G:C8 | 81:2:585:G:O5' | 2.63 | 0.51 |
| 81:2:882:C:H2' | 81:2:883:A:O4' | 2.11 | 0.51 |
| 1:5:1452:A:H2' | 1:5:1827:A:N3 | 2.26 | 0.51 |
| 1:5:2055:G:H2' | 1:5:2056:C:C6 | 2.46 | 0.51 |
| 1:5:2592:G:C6 | 1:5:2593:C:N4 | 2.79 | 0.51 |
| 1:5:482:G:H2' | 1:5:483:C:O4' | 2.11 | 0.51 |
| 1:5:504:A:N6 | 1:5:529:U:H5 | 2.07 | 0.51 |
| 1:5:646:U:H2' | 1:5:647:G:C8 | 2.46 | 0.51 |
| 5:BB:87:VAL:HG22 | 5:BB:110:LEU:CD2 | 2.41 | 0.51 |
| 6:CC:74:ILE:HD13 | 6:CC:94:CYS:SG | 2.50 | 0.51 |
| 24:VV:17:LEU:HD11 | 24:VV:98:ASN:HB3 | 1.92 | 0.51 |
| 24:VV:20:GLY:N | 24:VV:36:ILE:O | 2.44 | 0.51 |
| 83:1:53:GLU:HB3 | 83:1:54:ALA:C | 2.30 | 0.51 |
| 83:1:685:ARG:CB | 83:1:686:VAL:HA | 2.31 | 0.51 |
| 83:1:700:ARG:HG2 | 83:1:705:ILE:CD1 | 2.40 | 0.51 |
| 83:1:78:TYR:CG | 83:1:79:SER:HA | 2.46 | 0.51 |
| 81:2:431:G:C6 | 81:2:432:C:N3 | 2.79 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 57:J:170:GLY:CA | 81:2:510:A:H2' | 2.26 | 0.51 |
| 82:4:6120:U:C2' | 82:4:6127:C:H5'' | 2.39 | 0.51 |
| 82:4:6178:U:C5 | 82:4:6179:U:C5 | 2.98 | 0.51 |
| 1:5:1108:C:N4 | 1:5:1109:U:C4 | 2.79 | 0.51 |
| 1:5:2218:G:N2 | 1:5:2219:G:C5 | 2.78 | 0.51 |
| 1:5:3243:U:O2' | 1:5:3244:G:H4' | 2.10 | 0.51 |
| 1:5:370:U:O4 | 1:5:371:G:C6 | 2.64 | 0.51 |
| 4:AA:35:ALA:HA | 10:GG:35:ILE:HG23 | 1.92 | 0.51 |
| 10:GG:135:LEU:HA | 10:GG:196:VAL:HG21 | 1.93 | 0.51 |
| 13:JJ:49:LYS:HA | 13:JJ:64:LYS:HA | 1.91 | 0.51 |
| 83:1:583:HIS:HD1 | 83:1:704:GLN:HB3 | 1.74 | 0.51 |
| 83:1:726:GLU:HG3 | 83:1:727:PRO:HD2 | 1.93 | 0.51 |
| 81:2:1353:G:C2 | 81:2:1354:C:C2 | 2.99 | 0.51 |
| 82:4:6103:G:H2' | 82:4:6104:G:O4' | 2.10 | 0.51 |
| 1:5:2223:U:O2' | 82:4:6179:U:OP1 | 2.25 | 0.51 |
| 1:5:2807:G:N2 | 1:5:2808:C:C2 | 2.79 | 0.51 |
| 1:5:610:C:C2 | 1:5:611:C:C5 | 2.98 | 0.51 |
| 1:5:819:A:C5 | 1:5:820:C:H1' | 2.46 | 0.51 |
| 6:CC:349:ILE:HG13 | 6:CC:350:LYS:HB3 | 1.89 | 0.51 |
| 6:CC:349:ILE:CD1 | 6:CC:350:LYS:HA | 2.41 | 0.51 |
| 6:CC:37:SER:O | 6:CC:38:VAL:C | 2.49 | 0.51 |
| 17:OO:142[A]:LEU:HG | 17:OO:143[A]:SER:N | 2.25 | 0.51 |
| 48:A:185:ARG:HG3 | 69:V:45:ALA:HB3 | 1.92 | 0.51 |
| 83:1:155:VAL:HG21 | 83:1:185:VAL:HG11 | 1.92 | 0.51 |
| 83:1:157:ILE:CD1 | 83:1:211:PHE:HE1 | 2.22 | 0.51 |
| 83:1:383:SER:HA | 83:1:465:LYS:O | 2.10 | 0.51 |
| 83:1:576:LEU:CD2 | 83:1:587:TYR:HA | 2.41 | 0.51 |
| 81:2:1108:G:C4 | 81:2:1109:G:C8 | 2.99 | 0.51 |
| 81:2:1120:C:O2 | 81:2:1126:G:C2 | 2.64 | 0.51 |
| 81:2:585:G:C6 | 81:2:586:C:N4 | 2.78 | 0.51 |
| 81:2:888:U:H1' | 81:2:987:A:H4' | 1.91 | 0.51 |
| 1:5:1911:U:H2' | 1:5:1912:C:O4' | 2.11 | 0.51 |
| 1:5:3023:U:H3 | 1:5:3055:A:N6 | 2.06 | 0.51 |
| 1:5:3056:G:C6 | 1:5:3057:C:C4 | 2.99 | 0.51 |
| 1:5:3215:G:C2 | 1:5:3216:C:C2 | 2.99 | 0.51 |
| 1:5:65:A:C4 | 1:5:110:G:N7 | 2.79 | 0.51 |
| 5:BB:313:HIS:O | 5:BB:314:TYR:C | 2.46 | 0.51 |
| 17:OO:156[A]:LYS:C | 17:OO:158[A]:GLU:N | 2.64 | 0.51 |
| 83:1:519:LEU:HD13 | 83:1:521:TYR:HB3 | 1.93 | 0.51 |
| 50:C:82:LYS:HA | 50:C:83:ASP:CB | 2.40 | 0.51 |
| 8:EE:114:ARG:CG | 8:EE:115:ALA:H | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 17:OO:126[A]:ARG:NH1 | 17:OO:126[A]:ARG:HB3 | 2.26 | 0.51 |
| 81:2:1588:G:N2 | 81:2:1589:C:C2 | 2.79 | 0.51 |
| 81:2:1770:C:C6 | 81:2:1770:C:H5' | 2.46 | 0.51 |
| 82:4:6196:A:H2' | 82:4:6197:A:C8 | 2.46 | 0.51 |
| 1:5:1328:G:C6 | 1:5:1329:C:C4 | 2.99 | 0.51 |
| 1:5:1573:U:H3' | 1:5:1573:U:O2 | 2.11 | 0.51 |
| 1:5:3224:G:C2 | 1:5:3225:C:C2 | 2.99 | 0.51 |
| 1:5:486:U:O3' | 6:CC:343:LYS:O | 2.29 | 0.51 |
| 7:DD:39:GLN:HE21 | 7:DD:43:LYS:CD | 2.24 | 0.51 |
| 16:NN:143:ARG:NH1 | 16:NN:152:CYS:SG | 2.84 | 0.51 |
| 68:U:72:ASN:ND2 | 81:2:1427:G:N3 | 2.59 | 0.51 |
| 71:X:53:VAL:HG22 | 71:X:72:VAL:HG11 | 1.93 | 0.51 |
| 83:1:659:ILE:HD13 | 83:1:693:LEU:HD21 | 1.93 | 0.50 |
| 81:2:1471:U:O2 | 81:2:1471:U:C2' | 2.58 | 0.50 |
| 81:2:30:G:H2' | 81:2:31:C:O4' | 2.11 | 0.50 |
| 1:5:128:G:H2' | 1:5:129:C:O4' | 2.11 | 0.50 |
| 1:5:1300:U:O2' | 1:5:1301:A:OP1 | 2.23 | 0.50 |
| 1:5:1924:C:C4 | 1:5:2055:G:N1 | 2.76 | 0.50 |
| 1:5:2735:U:H2' | 1:5:2736:U:C6 | 2.47 | 0.50 |
| 1:5:2749:U:O2 | 1:5:2750:U:C2 | 2.63 | 0.50 |
| 1:5:3262:A:H2' | 1:5:3263:A:O4' | 2.10 | 0.50 |
| 5:BB:283:TYR:CZ | 5:BB:325:LYS:HG3 | 2.46 | 0.50 |
| 52:E:116:ASP:N | 52:E:117:GLU:HB2 | 2.26 | 0.50 |
| 9:FF:211:TRP:CE2 | 9:FF:216:LYS:HD2 | 2.47 | 0.50 |
| 10:GG:152:ILE:HG23 | 10:GG:162:VAL:HG21 | 1.93 | 0.50 |
| 14:LL:3:ILE:O | 14:LL:4:SER:OG | 2.19 | 0.50 |
| 17:OO:30[A]:ASN:O | 17:OO:32[A]:GLN:N | 2.41 | 0.50 |
| 19:QQ:122:ILE:HG23 | 19:QQ:126:GLN:HB2 | 1.93 | 0.50 |
| 20:RR:134:HIS:O | 20:RR:136:ARG:N | 2.43 | 0.50 |
| 81:2:1015:C:O2 | 81:2:1015:C:O4' | 2.28 | 0.50 |
| 81:2:1353:G:C6 | 81:2:1354:C:C4 | 2.99 | 0.50 |
| 81:2:886:A:H2 | 81:2:925:A:H2 | 1.35 | 0.50 |
| 82:4:6118:U:H2' | 82:4:6119:U:H4' | 1.93 | 0.50 |
| 3:8:8:C:HO2' | 3:8:9:A:H8 | 1.59 | 0.50 |
| 5:BB:215:ILE:HD12 | 5:BB:282:VAL:CG2 | 2.40 | 0.50 |
| 17:OO:28[A]:LEU:C | 17:OO:30[A]:ASN:N | 2.64 | 0.50 |
| 17:OO:76[A]:ALA:C | 17:OO:78[A]:SER:N | 2.64 | 0.50 |
| 81:2:1040:G:C6 | 81:2:1041:G:C6 | 2.99 | 0.50 |
| 81:2:1363:G:C2 | 81:2:1364:C:C4 | 2.98 | 0.50 |
| 81:2:864:A:N1 | 81:2:964:U:H5 | 2.09 | 0.50 |
| 1:5:1018:A:N3 | 1:5:2601:U:O2' | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|---------------------|--------------------------|-------------------|
| 1:5:618:A:C8 | 1:5:622:A:C6 | 2.99 | 0.50 |
| 1:5:995:G:N2 | 1:5:997:A:OP2 | 2.44 | 0.50 |
| 14:LL:27:ASP:O | 14:LL:28:GLN:C | 2.49 | 0.50 |
| 17:OO:126[A]:ARG:HD2 | 17:OO:136[A]:TYR:CG | 2.46 | 0.50 |
| 63:P:18:LYS:HA | 66:S:91:ASP:C | 2.32 | 0.50 |
| 64:Q:34:SER:HB2 | 64:Q:38:LEU:HD12 | 1.93 | 0.50 |
| 81:2:1673:C:N3 | 81:2:1725:G:C2 | 2.80 | 0.50 |
| 81:2:8:U:C4 | 81:2:1138:A:N6 | 2.79 | 0.50 |
| 1:5:2236:C:P | 82:4:6206:DG:OP2 | 2.67 | 0.50 |
| 1:5:1049:U:O2 | 1:5:1053:U:C2 | 2.64 | 0.50 |
| 1:5:1196:A:C3' | 1:5:1197:G:H5' | 2.41 | 0.50 |
| 1:5:1346:G:N1 | 1:5:1347:C:C4 | 2.80 | 0.50 |
| 1:5:1722:G:C6 | 1:5:1723:C:C4 | 3.00 | 0.50 |
| 1:5:1927:G:N1 | 1:5:2054:U:H2' | 2.27 | 0.50 |
| 1:5:2170:G:C2 | 1:5:2171:C:C2 | 3.00 | 0.50 |
| 1:5:2217:C:C5' | 1:5:2218:G:H5' | 2.41 | 0.50 |
| 1:5:2564:U:C4 | 1:5:2565:U:C4 | 2.99 | 0.50 |
| 1:5:3207:G:N2 | 1:5:3208:C:C2 | 2.79 | 0.50 |
| 2:7:12:U:OP2 | 2:7:68:C:O2' | 2.29 | 0.50 |
| 7:DD:165:GLY:O | 7:DD:169:GLY:N | 2.43 | 0.50 |
| 8:EE:126:LYS:N | 8:EE:126:LYS:CD | 2.74 | 0.50 |
| 53:F:53:VAL:HG13 | 53:F:133:GLN:HA | 1.93 | 0.50 |
| 81:2:1146:A:H2' | 81:2:1147:C:O4' | 2.11 | 0.50 |
| 1:5:2392:U:H2' | 1:5:2393:A:C8 | 2.47 | 0.50 |
| 1:5:3188:G:N2 | 1:5:3189:C:C2 | 2.79 | 0.50 |
| 1:5:3254:G:C2 | 1:5:3255:C:C2 | 3.00 | 0.50 |
| 4:AA:134:VAL:HG22 | 4:AA:150:LEU:HD23 | 1.94 | 0.50 |
| 49:B:103:MET:SD | 49:B:104:ASP:N | 2.83 | 0.50 |
| 5:BB:306:THR:HG22 | 5:BB:317:ILE:HB | 1.93 | 0.50 |
| 17:OO:143[A]:SER:C | 17:OO:145[A]:SER:N | 2.63 | 0.50 |
| 70:W:36:LYS:HB2 | 70:W:110:ILE:HD12 | 1.92 | 0.50 |
| 83:1:633:ILE:HG22 | 83:1:647:ILE:HG12 | 1.94 | 0.50 |
| 83:1:750:LYS:C | 83:1:751:ARG:CG | 2.77 | 0.50 |
| 81:2:17:C:O2' | 81:2:1136:A:N1 | 2.39 | 0.50 |
| 81:2:1671:G:C6 | 81:2:1672:C:C4 | 3.00 | 0.50 |
| 81:2:700:C:O2 | 81:2:739:G:C2 | 2.64 | 0.50 |
| 81:2:992:A:H5'' | 81:2:993:G:OP2 | 2.12 | 0.50 |
| 82:4:6178:U:C4 | 82:4:6198:A:N1 | 2.80 | 0.50 |
| 1:5:167:U:C5 | 1:5:168:U:C5 | 2.99 | 0.50 |
| 1:5:2824:G:N2 | 1:5:2825:C:C2 | 2.79 | 0.50 |
| 1:5:3055:A:C4' | 1:5:3055:A:C8 | 2.95 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:5:335:G:C2 | 1:5:336:A:C8 | 2.99 | 0.50 |
| 1:5:520:G:C2' | 1:5:521:U:H5' | 2.38 | 0.50 |
| 4:AA:110:GLY:HA2 | 81:2:922:A:H5'' | 1.94 | 0.50 |
| 17:OO:47[A]:GLU:O | 17:OO:48[A]:PHE:C | 2.50 | 0.50 |
| 83:1:576:LEU:HB3 | 83:1:585:ARG:HH21 | 1.76 | 0.50 |
| 81:2:1412:U:O4' | 81:2:1412:U:O2 | 2.28 | 0.50 |
| 81:2:1610:U:H3' | 81:2:1611:U:O2 | 2.12 | 0.50 |
| 1:5:1627:G:O4' | 1:5:1765:G:H2' | 2.12 | 0.50 |
| 1:5:2180:U:O4' | 1:5:2180:U:O2 | 2.29 | 0.50 |
| 1:5:2218:G:C4 | 1:5:2219:G:O4' | 2.64 | 0.50 |
| 2:7:25:G:C6 | 2:7:26:C:C4 | 3.00 | 0.50 |
| 5:BB:173:GLN:O | 5:BB:175:LYS:N | 2.45 | 0.50 |
| 7:DD:33:ARG:HE | 7:DD:37:VAL:HG21 | 1.77 | 0.50 |
| 12:II:65:LEU:HD11 | 12:II:91:VAL:CG1 | 2.41 | 0.50 |
| 17:OO:24[A]:VAL:CG1 | 17:OO:24[A]:VAL:O | 2.58 | 0.50 |
| 28:ZZ:61:LYS:O | 28:ZZ:65:ARG:N | 2.44 | 0.50 |
| 83:1:380:LEU:HD12 | 83:1:399:ARG:O | 2.10 | 0.50 |
| 81:2:273:G:C6 | 81:2:274:C:N4 | 2.80 | 0.50 |
| 81:2:902:U:O3' | 81:2:903:G:H3' | 2.11 | 0.50 |
| 82:4:6105:U:H2' | 82:4:6106:U:H5'' | 1.94 | 0.50 |
| 82:4:6121:A:C6 | 82:4:6158:A:N1 | 2.79 | 0.50 |
| 1:5:1108:C:C4 | 1:5:1109:U:C4 | 3.00 | 0.50 |
| 1:5:2503:G:H2' | 1:5:2504:A:O4' | 2.11 | 0.50 |
| 1:5:396:A:O2' | 1:5:399:A:OP1 | 2.22 | 0.50 |
| 4:AA:104:LEU:HB3 | 4:AA:146:THR:HG21 | 1.94 | 0.50 |
| 17:OO:141[A]:LYS:O | 17:OO:143[A]:SER:C | 2.51 | 0.50 |
| 17:OO:99[A]:ALA:C | 17:OO:101[A]:GLU:N | 2.64 | 0.50 |
| 20:RR:122:SER:OG | 20:RR:123:LEU:N | 2.44 | 0.50 |
| 20:RR:163:ARG:HG2 | 81:2:812:U:O2 | 2.11 | 0.50 |
| 81:2:39:A:O2' | 81:2:468:C:N4 | 2.45 | 0.50 |
| 1:5:1074:A:H3' | 1:5:1075:G:C5' | 2.41 | 0.50 |
| 1:5:114:A:H2' | 1:5:115:A:H5' | 1.92 | 0.50 |
| 1:5:1617:A:H2' | 1:5:1618:U:O4' | 2.12 | 0.50 |
| 1:5:1923:G:C8 | 1:5:1923:G:P | 3.04 | 0.50 |
| 1:5:221:A:C4 | 1:5:224:C:N4 | 2.80 | 0.50 |
| 1:5:2667:G:C2 | 1:5:2724:C:C2 | 3.00 | 0.50 |
| 1:5:2752:G:H2' | 1:5:2753:A:O4' | 2.12 | 0.50 |
| 1:5:842:U:H2' | 1:5:843:U:C6 | 2.46 | 0.50 |
| 1:5:882:C:H5'' | 4:AA:15:ILE:HD13 | 1.94 | 0.50 |
| 4:AA:200:ARG:O | 4:AA:201:GLY:C | 2.51 | 0.50 |
| 1:5:209:A:H2' | 6:CC:162:THR:HG21 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:HH:112:ILE:CD1 | 11:HH:161:ILE:HD11 | 2.41 | 0.50 |
| 58:K:46:LEU:HD13 | 58:K:66:TYR:CD2 | 2.47 | 0.50 |
| 17:OO:122[A]:PRO:C | 17:OO:124[A]:ALA:N | 2.65 | 0.50 |
| 17:OO:166[A]:ALA:C | 17:OO:168[A]:TYR:N | 2.64 | 0.50 |
| 83:1:682:ARG:CZ | 83:1:801:TRP:CE3 | 2.94 | 0.49 |
| 81:2:1661:G:C6 | 81:2:1662:C:C4 | 3.00 | 0.49 |
| 81:2:84:A:H2' | 81:2:85:A:O4' | 2.11 | 0.49 |
| 1:5:1174:A:N3 | 1:5:2823:U:O2' | 2.36 | 0.49 |
| 1:5:1266:G:C2 | 1:5:1267:C:C2 | 3.00 | 0.49 |
| 3:8:8:C:O2' | 3:8:9:A:H8 | 1.95 | 0.49 |
| 56:I:68:ALA:HB2 | 56:I:183:TYR:OH | 2.12 | 0.49 |
| 17:OO:174[A]:ALA:O | 17:OO:176[A]:ASN:N | 2.44 | 0.49 |
| 17:OO:5[A]:GLU:HA | 17:OO:5[A]:GLU:OE1 | 2.10 | 0.49 |
| 17:OO:79[A]:ARG:O | 17:OO:80[A]:ILE:C | 2.46 | 0.49 |
| 81:2:851:C:H2' | 81:2:852:G:O4' | 2.12 | 0.49 |
| 1:5:922:A:N3 | 1:5:1340:A:C2 | 2.80 | 0.49 |
| 1:5:1926:U:H2' | 1:5:1927:G:O5' | 2.12 | 0.49 |
| 1:5:2480:A:H5'' | 10:GG:248:ARG:NH1 | 2.26 | 0.49 |
| 8:EE:112:LYS:HD2 | 8:EE:113:GLN:N | 2.26 | 0.49 |
| 16:NN:74:PRO:O | 16:NN:75:VAL:O | 2.29 | 0.49 |
| 63:P:19:GLY:HA3 | 66:S:94:ASP:C | 2.33 | 0.49 |
| 24:VV:81:GLN:O | 24:VV:98:ASN:ND2 | 2.45 | 0.49 |
| 28:ZZ:53:VAL:HG13 | 28:ZZ:62:VAL:HG22 | 1.94 | 0.49 |
| 81:2:1084:G:N2 | 81:2:1086:A:H3' | 2.27 | 0.49 |
| 81:2:1349:G:N1 | 81:2:1374:C:C2 | 2.80 | 0.49 |
| 81:2:93:A:C6 | 81:2:397:G:C6 | 3.00 | 0.49 |
| 54:G:154:ARG:C | 81:2:78:A:H3' | 2.31 | 0.49 |
| 82:4:6074:A:H2' | 82:4:6075:A:O4' | 2.13 | 0.49 |
| 1:5:2055:G:H2' | 1:5:2056:C:N1 | 2.27 | 0.49 |
| 1:5:2154:G:O2' | 1:5:2283:U:OP2 | 2.29 | 0.49 |
| 1:5:2480:A:C3' | 1:5:2481:C:C4' | 2.84 | 0.49 |
| 4:AA:150:LEU:O | 4:AA:153:GLY:N | 2.43 | 0.49 |
| 5:BB:91:GLY:O | 5:BB:101:SER:HA | 2.12 | 0.49 |
| 5:BB:219:ALA:HB3 | 5:BB:329:PRO:HG2 | 1.94 | 0.49 |
| 6:CC:138:ARG:C | 6:CC:138:ARG:HD3 | 2.32 | 0.49 |
| 10:GG:152:ILE:CG2 | 10:GG:162:VAL:HG21 | 2.42 | 0.49 |
| 24:VV:74:MET:HE3 | 24:VV:102:ILE:HD13 | 1.94 | 0.49 |
| 26:XX:82:LEU:HD11 | 26:XX:126:LEU:HD21 | 1.93 | 0.49 |
| 83:1:44:GLY:HA3 | 83:1:45:ILE:HD13 | 1.95 | 0.49 |
| 81:2:69:G:C6 | 81:2:70:C:C4 | 3.01 | 0.49 |
| 1:5:2480:A:C2' | 1:5:2481:C:C4' | 2.88 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5:296:A:N3 | 1:5:299:G:O2' | 2.38 | 0.49 |
| 5:BB:29:VAL:HG11 | 5:BB:339:ARG:HD3 | 1.93 | 0.49 |
| 51:D:48:ILE:HD13 | 51:D:84:ILE:HG23 | 1.94 | 0.49 |
| 28:ZZ:46:ILE:HD12 | 28:ZZ:46:ILE:C | 2.33 | 0.49 |
| 28:ZZ:46:ILE:HD11 | 28:ZZ:49:TYR:CG | 2.48 | 0.49 |
| 83:1:681:MET:SD | 83:1:682:ARG:HB3 | 2.53 | 0.49 |
| 81:2:1278:C:H2' | 81:2:1279:C:O4' | 2.12 | 0.49 |
| 81:2:1671:G:C5 | 81:2:1672:C:C4 | 3.00 | 0.49 |
| 81:2:884:G:C2' | 81:2:885:U:C4' | 2.91 | 0.49 |
| 61:N:55:ARG:NH1 | 81:2:959:U:OP2 | 2.43 | 0.49 |
| 1:5:1753:G:C6 | 1:5:1754:C:C4 | 3.01 | 0.49 |
| 1:5:1925:G:N3 | 1:5:2056:C:C1' | 2.75 | 0.49 |
| 1:5:2406:G:C2 | 1:5:2479:U:O2 | 2.65 | 0.49 |
| 1:5:2540:A:H2' | 1:5:2540:A:N3 | 2.28 | 0.49 |
| 1:5:3170:G:H2' | 1:5:3171:U:O4' | 2.13 | 0.49 |
| 1:5:3252:G:C6 | 1:5:3253:C:C4 | 3.00 | 0.49 |
| 1:5:435:C:O2 | 1:5:598:G:C2 | 2.66 | 0.49 |
| 1:5:832:C:OP2 | 1:5:833:U:OP2 | 2.31 | 0.49 |
| 1:5:918:G:C6 | 1:5:919:C:N4 | 2.81 | 0.49 |
| 50:C:144:ILE:HG12 | 50:C:223:ILE:HG23 | 1.95 | 0.49 |
| 11:HH:75:ILE:HA | 11:HH:78:LEU:HD12 | 1.94 | 0.49 |
| 58:K:54:PHE:HB3 | 58:K:55:VAL:HG23 | 1.94 | 0.49 |
| 16:NN:59:PHE:CD2 | 16:NN:135:VAL:HG22 | 2.48 | 0.49 |
| 17:OO:166[A]:ALA:O | 17:OO:168[A]:TYR:N | 2.46 | 0.49 |
| 17:OO:62[A]:ALA:O | 17:OO:64[A]:ALA:N | 2.43 | 0.49 |
| 6:CC:290:ILE:HG23 | 19:QQ:35:PHE:CE2 | 2.47 | 0.49 |
| 70:W:74:VAL:O | 81:2:1099:G:O2' | 2.23 | 0.49 |
| 1:5:1338:G:HO2' | 1:5:1339:U:H6 | 1.58 | 0.49 |
| 1:5:1395:C:H2' | 1:5:1396:U:O4' | 2.13 | 0.49 |
| 1:5:1479:C:OP1 | 18:PP:127:ARG:NH2 | 2.46 | 0.49 |
| 1:5:187:A:C5 | 1:5:211:A:C2 | 3.01 | 0.49 |
| 1:5:2480:A:N7 | 1:5:2481:C:C5 | 2.79 | 0.49 |
| 1:5:2853:C:C2 | 1:5:2906:G:C2 | 3.00 | 0.49 |
| 1:5:3139:U:C3' | 1:5:3140:A:H5'' | 2.42 | 0.49 |
| 1:5:3234:G:C6 | 1:5:3235:A:C6 | 3.00 | 0.49 |
| 1:5:674:G:C2 | 1:5:675:C:C2 | 3.00 | 0.49 |
| 4:AA:55:GLY:O | 4:AA:56:ALA:HB3 | 2.12 | 0.49 |
| 50:C:95:THR:O | 81:2:1145:G:O2' | 2.31 | 0.49 |
| 83:1:133:GLU:OE2 | 83:1:136:CYS:CA | 2.56 | 0.49 |
| 81:2:1289:U:H2' | 81:2:1290:G:C8 | 2.47 | 0.49 |
| 81:2:332:A:C6 | 81:2:333:G:C6 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5:1120:G:N2 | 1:5:1126:C:C2 | 2.81 | 0.49 |
| 1:5:1722:G:C2 | 1:5:1723:C:C2 | 3.01 | 0.49 |
| 1:5:422:A:C2 | 1:5:2332:A:H4' | 2.48 | 0.49 |
| 1:5:674:G:C6 | 1:5:675:C:C4 | 3.00 | 0.49 |
| 5:BB:80:ASP:CG | 5:BB:314:TYR:OH | 2.51 | 0.49 |
| 6:CC:106:TRP:O | 16:NN:203:ARG:NH2 | 2.42 | 0.49 |
| 52:E:67:GLN:CA | 52:E:68:ARG:HB2 | 2.43 | 0.49 |
| 17:OO:166[A]:ALA:C | 17:OO:168[A]:TYR:H | 2.15 | 0.49 |
| 82:4:6120:U:H2' | 82:4:6120:U:O2 | 2.12 | 0.49 |
| 82:4:6199:A:N6 | 82:4:6200:A:N6 | 2.61 | 0.49 |
| 1:5:1791:C:O2' | 1:5:1792:A:H8 | 1.96 | 0.49 |
| 1:5:2840:A:H4' | 1:5:2840:A:OP1 | 2.12 | 0.49 |
| 1:5:3200:G:O6 | 1:5:3223:U:C4 | 2.65 | 0.49 |
| 1:5:858:G:C4 | 1:5:859:A:C8 | 3.01 | 0.49 |
| 8:EE:39:ILE:HG21 | 8:EE:162:PHE:CD2 | 2.48 | 0.49 |
| 17:OO:15[A]:HIS:C | 17:OO:16[A]:LEU:O | 2.51 | 0.49 |
| 71:X:41:SER:O | 71:X:43:PHE:N | 2.45 | 0.49 |
| 81:2:1188:A:N3 | 81:2:1193:A:O2' | 2.36 | 0.49 |
| 81:2:1560:G:C6 | 81:2:1561:C:C4 | 3.01 | 0.49 |
| 81:2:1586:G:N1 | 81:2:1587:C:C2 | 2.81 | 0.49 |
| 81:2:69:G:C2 | 81:2:70:C:C2 | 3.01 | 0.49 |
| 82:4:6189:G:O4' | 87:1:903:6EM:N7 | 2.46 | 0.49 |
| 1:5:2342:A:N3 | 1:5:2792:G:O2' | 2.37 | 0.49 |
| 1:5:2843:U:O2 | 1:5:2843:U:H2' | 2.13 | 0.49 |
| 1:5:3077:G:C2 | 1:5:3094:C:N3 | 2.80 | 0.49 |
| 23:UU:75:TYR:CZ | 23:UU:79:LEU:HD11 | 2.48 | 0.49 |
| 81:2:1080:A:C6 | 81:2:1090:A:C6 | 3.01 | 0.49 |
| 81:2:1162:A:N6 | 81:2:1163:G:C6 | 2.80 | 0.49 |
| 81:2:1739:U:H2' | 81:2:1740:U:O4' | 2.13 | 0.49 |
| 81:2:991:A:O2' | 81:2:1783:U:O2 | 2.24 | 0.49 |
| 81:2:22:A:C2 | 81:2:23:G:C5 | 3.01 | 0.49 |
| 81:2:594:G:C6 | 81:2:595:C:N4 | 2.81 | 0.49 |
| 81:2:628:U:O4 | 81:2:969:A:C5 | 2.65 | 0.49 |
| 82:4:6128:A:H2' | 82:4:6129:G:C4' | 2.42 | 0.49 |
| 82:4:6159:G:C2 | 82:4:6160:G:C5 | 3.00 | 0.49 |
| 1:5:1452:A:OP1 | 1:5:1452:A:C4' | 2.60 | 0.49 |
| 1:5:2036:U:C3' | 1:5:2049:G:O6 | 2.61 | 0.49 |
| 1:5:2182:A:H2' | 1:5:2183:A:C8 | 2.47 | 0.49 |
| 1:5:2203:G:C2 | 1:5:2204:C:C2 | 3.01 | 0.49 |
| 1:5:2173:C:O2 | 1:5:2208:G:C2 | 2.66 | 0.49 |
| 1:5:2217:C:H5'' | 1:5:2218:G:H5' | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5:2236:C:H2' | 1:5:2237:U:H6 | 1.78 | 0.49 |
| 1:5:2446:G:C2 | 1:5:2447:C:C2 | 3.01 | 0.49 |
| 1:5:2850:U:H2' | 1:5:2851:U:C6 | 2.48 | 0.49 |
| 1:5:590:G:C6 | 1:5:591:C:C4 | 3.01 | 0.49 |
| 1:5:770:G:C6 | 1:5:772:A:C4 | 3.00 | 0.49 |
| 1:5:987:C:O2 | 1:5:987:C:O2' | 2.30 | 0.49 |
| 17:OO:182[A]:LYS:C | 17:OO:184[A]:ALA:H | 2.16 | 0.49 |
| 81:2:1611:U:O2 | 81:2:1611:U:O4' | 2.30 | 0.48 |
| 54:G:136:LYS:HE3 | 81:2:65:A:H3' | 1.95 | 0.48 |
| 54:G:154:ARG:H | 81:2:78:A:C4' | 2.25 | 0.48 |
| 81:2:885:U:H3' | 81:2:886:A:H5'' | 1.88 | 0.48 |
| 81:2:991:A:N3 | 81:2:991:A:O4' | 2.45 | 0.48 |
| 1:5:2107:A:O3' | 1:5:2108:A:H2' | 2.13 | 0.48 |
| 1:5:2154:G:C2' | 1:5:2155:U:O5' | 2.61 | 0.48 |
| 1:5:2475:U:H2' | 1:5:2476:C:C6 | 2.48 | 0.48 |
| 1:5:2769:A:O2' | 1:5:2770:A:H2' | 2.12 | 0.48 |
| 1:5:3228:G:N2 | 1:5:3229:C:C2 | 2.81 | 0.48 |
| 1:5:436:A:C6 | 1:5:597:G:C2 | 3.01 | 0.48 |
| 1:5:843:U:N3 | 1:5:859:A:C2 | 2.81 | 0.48 |
| 1:5:849:G:H1' | 1:5:851:G:H21 | 1.77 | 0.48 |
| 4:AA:77:ILE:CD1 | 4:AA:128:ARG:HB3 | 2.43 | 0.48 |
| 49:B:99:ASN:O | 49:B:101:HIS:N | 2.46 | 0.48 |
| 1:5:664:A:N6 | 6:CC:48:GLN:NE2 | 2.61 | 0.48 |
| 8:EE:13:VAL:CG2 | 8:EE:14:PRO:HD3 | 2.34 | 0.48 |
| 22:TT:63:VAL:HB | 22:TT:75:ILE:CD1 | 2.43 | 0.48 |
| 83:1:463:LEU:CD1 | 83:1:467:GLY:HA3 | 2.33 | 0.48 |
| 81:2:991:A:C2 | 81:2:1011:U:O4 | 2.66 | 0.48 |
| 81:2:406:A:H2' | 81:2:407:C:C6 | 2.49 | 0.48 |
| 81:2:922:A:C2 | 81:2:923:A:C6 | 3.00 | 0.48 |
| 81:2:966:A:H2' | 81:2:967:U:O4' | 2.13 | 0.48 |
| 1:5:1075:G:H2' | 1:5:1076:A:C8 | 2.48 | 0.48 |
| 1:5:226:C:H2' | 1:5:227:G:O4' | 2.12 | 0.48 |
| 1:5:2915:G:N2 | 1:5:2916:C:C2 | 2.82 | 0.48 |
| 7:DD:111:GLN:HE22 | 7:DD:251:PRO:HD2 | 1.78 | 0.48 |
| 11:HH:41:ILE:HD11 | 11:HH:67:ALA:CB | 2.42 | 0.48 |
| 50:C:153:LEU:HD22 | 57:J:94:ASP:HB3 | 1.94 | 0.48 |
| 2:7:28:C:OP1 | 13:JJ:137:ARG:NH1 | 2.46 | 0.48 |
| 16:NN:104:GLU:HA | 16:NN:160:GLU:HG3 | 1.95 | 0.48 |
| 81:2:1440:U:N3 | 81:2:1441:U:C4 | 2.81 | 0.48 |
| 24:VV:67:PRO:HG3 | 81:2:1657:A:O2' | 2.13 | 0.48 |
| 82:4:6044:G:C6 | 82:4:6045:C:C4 | 3.02 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:5:2236:C:OP2 | 82:4:6206:DG:OP2 | 2.31 | 0.48 |
| 1:5:1925:G:N7 | 1:5:2057:A:C4 | 2.82 | 0.48 |
| 1:5:2203:G:C6 | 1:5:2204:C:C4 | 3.01 | 0.48 |
| 1:5:2480:A:N6 | 1:5:2481:C:N4 | 2.60 | 0.48 |
| 1:5:548:G:N2 | 1:5:549:C:C2 | 2.81 | 0.48 |
| 48:A:33:GLN:N | 48:A:34:GLU:HB2 | 2.28 | 0.48 |
| 4:AA:80:GLU:CG | 4:AA:170:ALA:HA | 2.43 | 0.48 |
| 1:5:666:A:O2' | 6:CC:234:GLY:HA3 | 2.13 | 0.48 |
| 17:OO:161[A]:ARG:CG | 17:OO:162[A]:LYS:H | 2.16 | 0.48 |
| 17:OO:94[A]:ALA:C | 17:OO:96[A]:GLY:N | 2.54 | 0.48 |
| 63:P:43:ARG:NH1 | 81:2:1549:U:OP2 | 2.46 | 0.48 |
| 18:PP:83:TRP:O | 18:PP:85:ALA:N | 2.46 | 0.48 |
| 71:X:53:VAL:HG13 | 71:X:72:VAL:HG13 | 1.95 | 0.48 |
| 83:1:705:ILE:C | 83:1:708:THR:HG22 | 2.33 | 0.48 |
| 81:2:1277:G:C2 | 81:2:1278:C:C2 | 3.01 | 0.48 |
| 81:2:1558:U:O4' | 81:2:1558:U:O2 | 2.30 | 0.48 |
| 81:2:591:G:H2' | 81:2:592:U:O4' | 2.13 | 0.48 |
| 1:5:1032:A:C2 | 1:5:1033:A:C4 | 3.01 | 0.48 |
| 1:5:1111:G:N2 | 1:5:1112:C:C2 | 2.81 | 0.48 |
| 1:5:1925:G:C6 | 1:5:2057:A:C5 | 3.01 | 0.48 |
| 1:5:2237:U:H3' | 1:5:2238:U:H5' | 1.94 | 0.48 |
| 1:5:2530:A:O2' | 1:5:2531:A:H5'' | 2.14 | 0.48 |
| 1:5:987:C:O2' | 1:5:988:C:O5' | 2.31 | 0.48 |
| 55:H:70:TYR:O | 55:H:74:GLN:N | 2.46 | 0.48 |
| 18:PP:36:ILE:HG23 | 18:PP:114:VAL:HG11 | 1.95 | 0.48 |
| 18:PP:36:ILE:HD12 | 18:PP:48:LEU:HD11 | 1.95 | 0.48 |
| 22:TT:95:HIS:C | 22:TT:96:ILE:HD12 | 2.32 | 0.48 |
| 71:X:63:GLN:O | 71:X:65:ASN:N | 2.47 | 0.48 |
| 81:2:1170:A:H2' | 81:2:1171:G:C8 | 2.47 | 0.48 |
| 81:2:1560:G:C2 | 81:2:1561:C:C2 | 3.01 | 0.48 |
| 81:2:626:C:H2' | 81:2:627:G:O4' | 2.13 | 0.48 |
| 82:4:6119:U:C5' | 82:4:6120:U:H5'' | 2.35 | 0.48 |
| 1:5:2444:G:C2 | 1:5:2445:C:C2 | 3.02 | 0.48 |
| 1:5:885:A:C2 | 4:AA:204:MET:SD | 3.06 | 0.48 |
| 2:7:112:G:H2' | 2:7:113:C:C6 | 2.49 | 0.48 |
| 3:8:56:G:C2 | 3:8:57:C:C2 | 3.01 | 0.48 |
| 17:OO:16[A]:LEU:HD21 | 17:OO:126[A]:ARG:HG3 | 1.94 | 0.48 |
| 18:PP:64:ASN:ND2 | 18:PP:80:LYS:HE3 | 2.29 | 0.48 |
| 22:TT:45:ASN:O | 22:TT:46:GLY:C | 2.52 | 0.48 |
| 83:1:576:LEU:HD21 | 83:1:587:TYR:HD1 | 0.52 | 0.48 |
| 81:2:1306:U:O2 | 81:2:1306:U:O4' | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|--------------------|--------------------------|-------------------|
| 81:2:52:U:H2' | 81:2:53:G:C8 | 2.48 | 0.48 |
| 81:2:885:U:C3' | 81:2:886:A:C5' | 2.85 | 0.48 |
| 49:B:117:TRP:HD1 | 81:2:931:U:OP2 | 1.96 | 0.48 |
| 1:5:1277:G:N2 | 1:5:1278:G:N7 | 2.56 | 0.48 |
| 1:5:1717:G:C6 | 1:5:1718:A:C6 | 3.02 | 0.48 |
| 1:5:1729:C:C2 | 1:5:1735:G:N1 | 2.82 | 0.48 |
| 1:5:193:C:C2 | 1:5:203:G:N2 | 2.82 | 0.48 |
| 1:5:2911:G:C2' | 5:BB:254:ALA:HB1 | 2.43 | 0.48 |
| 17:OO:125[A]:LEU:HD22 | 17:OO:125[A]:LEU:H | 1.79 | 0.48 |
| 83:1:204:PRO:CG | 83:1:245:TRP:CE2 | 2.87 | 0.48 |
| 81:2:1292:U:O4 | 81:2:1293:G:C5 | 2.67 | 0.48 |
| 81:2:1300:U:H2' | 81:2:1301:U:O4' | 2.13 | 0.48 |
| 81:2:53:G:C6 | 81:2:54:C:C4 | 3.01 | 0.48 |
| 81:2:556:G:C6 | 81:2:558:C:N4 | 2.82 | 0.48 |
| 81:2:931:U:H1' | 81:2:932:A:C2 | 2.49 | 0.48 |
| 82:4:6107:A:H2' | 82:4:6108:G:C8 | 2.48 | 0.48 |
| 1:5:954:A:C2 | 1:5:1072:G:C2 | 3.02 | 0.48 |
| 1:5:2036:U:H2' | 1:5:2049:G:O6 | 2.14 | 0.48 |
| 1:5:2159:U:H2' | 1:5:2160:U:O4' | 2.14 | 0.48 |
| 1:5:1420:A:C2 | 1:5:2325:A:C4 | 3.01 | 0.48 |
| 1:5:2479:U:N3 | 1:5:2480:A:C8 | 2.81 | 0.48 |
| 4:AA:9:ARG:O | 4:AA:11:GLY:N | 2.47 | 0.48 |
| 5:BB:3:HIS:O | 5:BB:5:LYS:N | 2.46 | 0.48 |
| 83:1:47:SER:CA | 83:1:48:ALA:HB3 | 2.44 | 0.48 |
| 81:2:1000:A:H3' | 81:2:1001:G:C8 | 2.48 | 0.48 |
| 81:2:1451:G:H2' | 81:2:1452:G:O4' | 2.14 | 0.48 |
| 81:2:585:G:N2 | 81:2:586:C:C2 | 2.81 | 0.48 |
| 1:5:1055:A:H2' | 1:5:1056:A:C8 | 2.49 | 0.48 |
| 1:5:2862:C:O2 | 1:5:2876:G:C2 | 2.67 | 0.48 |
| 4:AA:27:ALA:O | 4:AA:128:ARG:NH1 | 2.47 | 0.48 |
| 56:I:142:ARG:NH2 | 81:2:196:A:N1 | 2.62 | 0.48 |
| 62:O:31:THR:HG22 | 62:O:38:THR:HA | 1.96 | 0.48 |
| 83:1:103:ILE:CD1 | 83:1:118:ALA:HB1 | 2.44 | 0.48 |
| 81:2:1363:G:C6 | 81:2:1364:C:N4 | 2.82 | 0.48 |
| 81:2:1417:G:C6 | 81:2:1418:C:N3 | 2.82 | 0.48 |
| 81:2:884:G:C8 | 81:2:885:U:C6 | 3.02 | 0.48 |
| 82:4:6170:C:H2' | 82:4:6171:U:O4' | 2.14 | 0.48 |
| 1:5:1261:A:H2' | 1:5:1262:A:O4' | 2.13 | 0.48 |
| 1:5:2167:A:N9 | 1:5:2238:U:C2 | 2.82 | 0.48 |
| 1:5:2444:G:C6 | 1:5:2445:C:C4 | 3.02 | 0.48 |
| 1:5:2506:U:O2 | 1:5:2506:U:C2' | 2.62 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 3:8:75:G:C2 | 3:8:76:C:C2 | 3.02 | 0.48 |
| 50:C:234:LEU:O | 50:C:235:TRP:C | 2.52 | 0.48 |
| 6:CC:74:ILE:CG2 | 6:CC:88:ALA:HB1 | 2.44 | 0.48 |
| 10:GG:159:ILE:HD12 | 16:NN:22:LEU:HD21 | 1.94 | 0.48 |
| 59:L:88:ARG:NH2 | 81:2:304:C:O3' | 2.47 | 0.48 |
| 69:V:53:TYR:OH | 69:V:76:ASP:HB2 | 2.13 | 0.48 |
| 71:X:43:PHE:CZ | 71:X:122:PHE:CD1 | 3.02 | 0.48 |
| 82:4:6182:A:P | 83:1:585:ARG:NH1 | 2.86 | 0.48 |
| 64:Q:139:GLN:HA | 81:2:1577:U:O2' | 2.13 | 0.48 |
| 81:2:958:U:H5' | 81:2:958:U:O2 | 2.14 | 0.48 |
| 1:5:1469:A:H2' | 1:5:1470:C:C6 | 2.48 | 0.48 |
| 1:5:1467:C:C2 | 1:5:1492:G:N2 | 2.82 | 0.48 |
| 3:8:107:G:N2 | 3:8:108:C:C2 | 2.82 | 0.48 |
| 12:II:149:ILE:HD11 | 12:II:167:ILE:HD11 | 1.94 | 0.48 |
| 59:L:91:LEU:HD13 | 59:L:100:TYR:CG | 2.49 | 0.48 |
| 67:T:48:GLN:OE1 | 81:2:1529:G:N2 | 2.44 | 0.48 |
| 70:W:95:PRO:HD2 | 70:W:130:TYR:HB3 | 1.96 | 0.48 |
| 83:1:567:VAL:HG13 | 83:1:684:VAL:HG22 | 1.95 | 0.47 |
| 81:2:1499:C:C2 | 81:2:1505:G:N2 | 2.82 | 0.47 |
| 81:2:1589:C:C2 | 81:2:1590:A:C8 | 3.01 | 0.47 |
| 81:2:50:C:O2 | 81:2:429:G:C2 | 2.66 | 0.47 |
| 81:2:53:G:C2 | 81:2:54:C:C2 | 3.02 | 0.47 |
| 1:5:1755:G:H2' | 1:5:1756:A:C8 | 2.48 | 0.47 |
| 1:5:1923:G:N1 | 1:5:1925:G:C8 | 2.81 | 0.47 |
| 1:5:2422:U:H4' | 1:5:2423:G:OP1 | 2.14 | 0.47 |
| 1:5:2481:C:OP1 | 10:GG:245:ILE:CG1 | 2.60 | 0.47 |
| 1:5:2694:C:N4 | 1:5:2696:G:C6 | 2.82 | 0.47 |
| 1:5:610:C:H1' | 1:5:611:C:C6 | 2.49 | 0.47 |
| 1:5:658:G:C2 | 1:5:669:C:C2 | 3.03 | 0.47 |
| 1:5:947:U:H2' | 1:5:948:C:O4' | 2.14 | 0.47 |
| 48:A:43:ASP:CG | 65:R:126:ALA:HB1 | 2.35 | 0.47 |
| 9:FF:220:PHE:O | 9:FF:221:ILE:HG22 | 2.12 | 0.47 |
| 62:O:20:PHE:HB3 | 62:O:27:PHE:HB2 | 1.95 | 0.47 |
| 17:OO:17[A]:LEU:HG | 17:OO:18[A]:GLY:N | 2.29 | 0.47 |
| 17:OO:77[A]:PRO:HG2 | 17:OO:148[A]:TRP:CE2 | 2.49 | 0.47 |
| 82:4:6191:A:H2' | 82:4:6192:G:O4' | 2.14 | 0.47 |
| 1:5:1515:G:C2 | 1:5:1521:C:C2 | 3.02 | 0.47 |
| 1:5:1860:A:H8 | 1:5:1860:A:H5'' | 1.79 | 0.47 |
| 1:5:2238:U:H2' | 1:5:2239:A:O5' | 2.14 | 0.47 |
| 1:5:2242:G:N2 | 1:5:2280:G:H2' | 2.29 | 0.47 |
| 1:5:2242:G:H1' | 1:5:2280:G:N1 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 57:J:37:LYS:N | 57:J:41:GLU:OE1 | 2.44 | 0.47 |
| 15:MM:32:LEU:HD11 | 15:MM:94:TRP:CG | 2.49 | 0.47 |
| 17:OO:182[A]:LYS:CA | 17:OO:185[A]:THR:HG22 | 2.43 | 0.47 |
| 64:Q:52:LEU:HD22 | 64:Q:60:PHE:CZ | 2.49 | 0.47 |
| 48:A:4:PRO:HD3 | 69:V:39:VAL:HG11 | 1.95 | 0.47 |
| 83:1:463:LEU:CD1 | 83:1:467:GLY:CA | 2.87 | 0.47 |
| 81:2:1333:U:H2' | 81:2:1334:U:O4' | 2.13 | 0.47 |
| 81:2:642:G:C2 | 81:2:692:C:O2 | 2.68 | 0.47 |
| 81:2:849:A:C2 | 81:2:850:U:C2 | 3.02 | 0.47 |
| 81:2:980:U:H2' | 81:2:981:U:C6 | 2.48 | 0.47 |
| 1:5:1927:G:N1 | 1:5:2055:G:O4' | 2.47 | 0.47 |
| 1:5:2446:G:C6 | 1:5:2447:C:C4 | 3.02 | 0.47 |
| 1:5:3266:C:H5'' | 18:PP:71:ALA:HB1 | 1.96 | 0.47 |
| 1:5:520:G:H2' | 1:5:521:U:H5'' | 1.96 | 0.47 |
| 1:5:918:G:N2 | 1:5:919:C:C2 | 2.82 | 0.47 |
| 6:CC:187:LEU:HD22 | 6:CC:193:LYS:HE3 | 1.96 | 0.47 |
| 70:W:73:GLY:HA3 | 70:W:128:PHE:CZ | 2.49 | 0.47 |
| 1:5:1600:C:OP1 | 28:ZZ:69:LYS:HB2 | 2.15 | 0.47 |
| 83:1:189:VAL:HG11 | 83:1:201:GLN:HA | 1.96 | 0.47 |
| 83:1:681:MET:CB | 83:1:682:ARG:HG3 | 2.44 | 0.47 |
| 81:2:1126:G:C6 | 81:2:1127:C:C4 | 3.03 | 0.47 |
| 81:2:1396:U:H3' | 81:2:1397:C:H5' | 1.95 | 0.47 |
| 82:4:6105:U:C2' | 82:4:6106:U:H5'' | 2.45 | 0.47 |
| 82:4:6120:U:C6 | 82:4:6127:C:C5' | 2.97 | 0.47 |
| 1:5:1630:G:H2' | 1:5:1631:G:C8 | 2.49 | 0.47 |
| 1:5:172:A:N3 | 1:5:247:A:C6 | 2.82 | 0.47 |
| 1:5:1797:A:H2' | 1:5:1798:G:O4' | 2.14 | 0.47 |
| 1:5:292:U:C4 | 1:5:293:C:C5 | 3.02 | 0.47 |
| 1:5:2995:A:H2' | 1:5:2996:G:O4' | 2.13 | 0.47 |
| 1:5:3296:G:N2 | 1:5:3347:C:C2 | 2.82 | 0.47 |
| 1:5:33:G:N1 | 1:5:50:U:OP2 | 2.38 | 0.47 |
| 1:5:520:G:C2' | 1:5:521:U:C5' | 2.91 | 0.47 |
| 1:5:523:G:H2' | 1:5:524:A:C8 | 2.49 | 0.47 |
| 57:J:108:ARG:NH2 | 57:J:145:SER:OG | 2.47 | 0.47 |
| 17:OO:111[A]:PRO:HA | 17:OO:114[A]:ASP:OD1 | 2.14 | 0.47 |
| 83:1:519:LEU:HG | 83:1:531:ALA:CB | 2.44 | 0.47 |
| 83:1:578:LYS:O | 83:1:579:SER:C | 2.53 | 0.47 |
| 81:2:1147:C:O2' | 81:2:1763:A:N1 | 2.44 | 0.47 |
| 81:2:30:G:C6 | 81:2:31:C:C4 | 3.02 | 0.47 |
| 54:G:175:ILE:HG22 | 81:2:78:A:N3 | 2.28 | 0.47 |
| 1:5:101:G:H2' | 1:5:102:C:O4' | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------------|--------------------------|-------------------|
| 1:5:118:U:O2 | 1:5:121:A:H5' | 2.14 | 0.47 |
| 1:5:1700:A:H2' | 1:5:1701:G:O4' | 2.14 | 0.47 |
| 1:5:185:C:C2 | 1:5:232:G:C2 | 3.02 | 0.47 |
| 1:5:2170:G:C6 | 1:5:2171:C:C4 | 3.02 | 0.47 |
| 1:5:2215:G:N2 | 1:5:2216:G:C4 | 2.83 | 0.47 |
| 1:5:185:C:C2 | 1:5:232:G:N1 | 2.83 | 0.47 |
| 1:5:1105:G:O2' | 1:5:2610:A:N3 | 2.41 | 0.47 |
| 1:5:2979:A:N1 | 1:5:3011:C:O2' | 2.35 | 0.47 |
| 1:5:435:C:H2' | 1:5:436:A:H8 | 1.79 | 0.47 |
| 5:BB:324:LEU:HD13 | 5:BB:328:ILE:CD1 | 2.45 | 0.47 |
| 57:J:41:GLU:OE2 | 57:J:108:ARG:NH2 | 2.47 | 0.47 |
| 22:TT:79:MET:HB2 | 22:TT:84:TYR:CE1 | 2.49 | 0.47 |
| 83:1:701:GLY:HA3 | 83:1:703:GLY:N | 2.29 | 0.47 |
| 81:2:1437:C:H2' | 81:2:1438:C:H6 | 1.80 | 0.47 |
| 81:2:1672:C:H2' | 81:2:1673:C:C6 | 2.49 | 0.47 |
| 81:2:820:U:H2' | 81:2:821:U:C6 | 2.49 | 0.47 |
| 81:2:935:G:C6 | 81:2:936:C:C4 | 3.03 | 0.47 |
| 1:5:1266:G:C6 | 1:5:1267:C:C4 | 3.01 | 0.47 |
| 1:5:1283:C:H5'' | 1:5:1284:G:OP2 | 2.15 | 0.47 |
| 1:5:1753:G:C2 | 1:5:1754:C:C2 | 3.02 | 0.47 |
| 1:5:2238:U:H2' | 1:5:2239:A:C4' | 2.44 | 0.47 |
| 5:BB:252:ILE:CG2 | 5:BB:260:VAL:HG13 | 2.44 | 0.47 |
| 6:CC:41:SER:HB3 | 6:CC:111:VAL:HG11 | 1.97 | 0.47 |
| 17:OO:110[A]:PRO:O | 17:OO:111[A]:PRO:C | 2.53 | 0.47 |
| 17:OO:42[A]:LEU:CB | 17:OO:139[A]:LEU:HD22 | 2.44 | 0.47 |
| 9:FF:101:GLN:HG3 | 19:QQ:6:THR:HG22 | 1.96 | 0.47 |
| 1:5:1442:U:OP1 | 20:RR:5:ARG:NH1 | 2.48 | 0.47 |
| 1:5:3019:U:H1' | 24:VV:92:PHE:CZ | 2.48 | 0.47 |
| 83:1:643:PRO:O | 83:1:683:SER:HA | 2.14 | 0.47 |
| 81:2:1277:G:C6 | 81:2:1278:C:C4 | 3.03 | 0.47 |
| 81:2:1316:C:H2' | 81:2:1317:G:O4' | 2.14 | 0.47 |
| 81:2:1586:G:C2 | 81:2:1587:C:C2 | 3.02 | 0.47 |
| 82:4:6178:U:N3 | 82:4:6198:A:C2 | 2.81 | 0.47 |
| 1:5:1419:U:C5 | 1:5:2324:G:C2 | 3.02 | 0.47 |
| 1:5:1751:C:H2' | 1:5:1752:C:C6 | 2.50 | 0.47 |
| 1:5:1786:G:C4 | 1:5:1787:U:C5 | 3.03 | 0.47 |
| 1:5:3040:C:H2' | 1:5:3041:A:O4' | 2.14 | 0.47 |
| 1:5:3128:C:H2' | 1:5:3129:U:C6 | 2.48 | 0.47 |
| 6:CC:208:VAL:CG1 | 6:CC:230:VAL:HG22 | 2.44 | 0.47 |
| 7:DD:148:VAL:HG21 | 7:DD:153:THR:CG2 | 2.44 | 0.47 |
| 21:SS:155:ARG:HD3 | 21:SS:172:TYR:CD1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 71:X:69:ARG:NH1 | 71:X:116:ASP:OD2 | 2.47 | 0.47 |
| 83:1:644:ASN:OD1 | 83:1:681:MET:SD | 2.73 | 0.47 |
| 50:C:173:ARG:HD2 | 81:2:1096:U:H1' | 1.97 | 0.47 |
| 65:R:10:LYS:NZ | 81:2:1315:G:O2' | 2.46 | 0.47 |
| 81:2:1578:C:H2' | 81:2:1579:C:O4' | 2.15 | 0.47 |
| 81:2:1670:G:C2 | 81:2:1671:G:C5 | 3.02 | 0.47 |
| 81:2:394:U:H2' | 81:2:395:G:O4' | 2.15 | 0.47 |
| 81:2:922:A:N1 | 81:2:923:A:C6 | 2.83 | 0.47 |
| 81:2:876:G:N1 | 81:2:951:A:C2 | 2.83 | 0.47 |
| 1:5:1196:A:H2' | 1:5:1197:G:H5' | 1.96 | 0.47 |
| 1:5:1923:G:P | 1:5:1923:G:H8 | 2.37 | 0.47 |
| 1:5:2149:G:C2 | 1:5:2150:C:N3 | 2.83 | 0.47 |
| 1:5:2482:U:H4' | 1:5:2483:U:OP1 | 2.15 | 0.47 |
| 1:5:2915:G:H4' | 1:5:2915:G:OP2 | 2.15 | 0.47 |
| 1:5:3056:G:C5 | 1:5:3057:C:C4 | 3.03 | 0.47 |
| 1:5:469:A:O2' | 1:5:3241:A:N1 | 2.39 | 0.47 |
| 1:5:3260:A:O2' | 5:BB:132:LYS:NZ | 2.40 | 0.47 |
| 5:BB:283:TYR:OH | 5:BB:325:LYS:HG3 | 2.15 | 0.47 |
| 6:CC:232:SER:OG | 6:CC:233:LEU:N | 2.48 | 0.47 |
| 11:HH:170:LYS:HB3 | 11:HH:175:PHE:CD2 | 2.50 | 0.47 |
| 62:O:40:ALA:HB3 | 62:O:67:VAL:HG22 | 1.96 | 0.47 |
| 19:QQ:32:LEU:HD23 | 19:QQ:33:TYR:N | 2.30 | 0.47 |
| 22:TT:80:VAL:HG11 | 22:TT:85:LEU:HD12 | 1.96 | 0.47 |
| 83:1:462:PHE:O | 83:1:463:LEU:CD2 | 2.63 | 0.47 |
| 81:2:1015:C:H2' | 81:2:1016:U:O4' | 2.15 | 0.47 |
| 81:2:1454:C:O4' | 81:2:1454:C:O2 | 2.31 | 0.47 |
| 81:2:1620:G:C2 | 81:2:1621:C:C2 | 3.03 | 0.47 |
| 81:2:1153:G:C2 | 81:2:1623:C:N3 | 2.83 | 0.47 |
| 81:2:623:G:C2 | 81:2:624:C:C2 | 3.03 | 0.47 |
| 1:5:1145:G:N2 | 1:5:1146:C:C2 | 2.82 | 0.47 |
| 1:5:1456:G:HO2' | 1:5:1843:A:HO2' | 1.60 | 0.47 |
| 1:5:170:G:H2' | 1:5:170:G:N3 | 2.30 | 0.47 |
| 1:5:852:C:H1' | 1:5:1819:A:C8 | 2.50 | 0.47 |
| 1:5:3042:G:C2 | 1:5:3043:G:C8 | 3.03 | 0.47 |
| 1:5:597:G:C2 | 1:5:598:G:C8 | 3.03 | 0.47 |
| 54:G:87:ARG:NH2 | 81:2:159:C:OP1 | 2.48 | 0.47 |
| 56:I:160:GLN:HB3 | 56:I:166:LEU:HA | 1.96 | 0.47 |
| 57:J:66:ASP:HB3 | 57:J:67:PRO:CD | 2.45 | 0.47 |
| 17:OO:13[A]:LYS:CD | 17:OO:38[A]:ARG:NH2 | 2.59 | 0.47 |
| 83:1:28:VAL:C | 83:1:30:HIS:H | 2.19 | 0.47 |
| 83:1:750:LYS:O | 83:1:751:ARG:CB | 2.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 81:2:1014:U:H2' | 81:2:1015:C:O2 | 2.15 | 0.47 |
| 81:2:1782:C:H2' | 81:2:1783:U:H6 | 1.79 | 0.47 |
| 81:2:291:U:H2' | 81:2:292:U:C6 | 2.50 | 0.47 |
| 81:2:30:G:C2 | 81:2:31:C:C2 | 3.03 | 0.47 |
| 81:2:900:G:N1 | 81:2:901:G:C6 | 2.83 | 0.47 |
| 1:5:1624:G:C8 | 1:5:1624:G:H5'' | 2.48 | 0.47 |
| 1:5:1845:U:H6 | 1:5:1845:U:H5'' | 1.80 | 0.47 |
| 3:8:68:G:H2' | 3:8:69:U:O4' | 2.15 | 0.47 |
| 9:FF:84:VAL:HA | 9:FF:110:SER:O | 2.14 | 0.47 |
| 17:OO:86[A]:ARG:CG | 17:OO:100[A]:LEU:CD1 | 2.93 | 0.47 |
| 19:QQ:36:LEU:O | 19:QQ:37:ALA:C | 2.53 | 0.47 |
| 72:Y:29:HIS:O | 72:Y:30:PRO:C | 2.54 | 0.47 |
| 83:1:547:HIS:O | 83:1:549:HIS:N | 2.48 | 0.47 |
| 83:1:721:ASP:H | 83:1:722:PRO:HD2 | 1.79 | 0.47 |
| 52:E:148:ARG:NE | 81:2:124:A:O2' | 2.48 | 0.47 |
| 81:2:1499:C:C2 | 81:2:1505:G:C2 | 3.03 | 0.47 |
| 81:2:1540:G:O2' | 81:2:1541:A:O4' | 2.31 | 0.47 |
| 81:2:1602:U:C4 | 81:2:1603:G:N7 | 2.83 | 0.47 |
| 1:5:1386:U:C4 | 1:5:1387:A:C6 | 3.02 | 0.47 |
| 1:5:1923:G:C2 | 1:5:1925:G:N7 | 2.82 | 0.47 |
| 52:E:31:PRO:HG2 | 52:E:38:LEU:HD22 | 1.97 | 0.47 |
| 10:GG:131:VAL:HG11 | 10:GG:188:LEU:CD1 | 2.45 | 0.47 |
| 58:K:42:VAL:HG12 | 58:K:46:LEU:HD12 | 1.97 | 0.47 |
| 16:NN:189:LYS:O | 16:NN:190:THR:C | 2.53 | 0.47 |
| 63:P:121:ILE:HD11 | 66:S:125:ILE:HD13 | 1.96 | 0.47 |
| 83:1:659:ILE:HD11 | 83:1:693:LEU:HD21 | 1.97 | 0.46 |
| 81:2:1091:A:C5 | 81:2:1093:G:C8 | 3.03 | 0.46 |
| 81:2:1497:G:C6 | 81:2:1498:C:C4 | 3.03 | 0.46 |
| 81:2:1603:G:C6 | 81:2:1604:C:C4 | 3.03 | 0.46 |
| 1:5:173:G:C4 | 1:5:174:C:C5 | 3.03 | 0.46 |
| 1:5:2249:A:C3' | 1:5:2250:A:H5' | 2.45 | 0.46 |
| 1:5:3051:G:C6 | 1:5:3052:C:C4 | 3.03 | 0.46 |
| 1:5:466:G:C6 | 1:5:467:C:C4 | 3.03 | 0.46 |
| 1:5:2915:G:C5 | 5:BB:251:CYS:SG | 3.08 | 0.46 |
| 6:CC:74:ILE:HD11 | 6:CC:93:MET:CE | 2.45 | 0.46 |
| 6:CC:77:VAL:O | 6:CC:86:GLY:N | 2.48 | 0.46 |
| 55:H:173:TYR:CE1 | 55:H:177:THR:HG21 | 2.51 | 0.46 |
| 17:OO:159[A]:GLU:O | 17:OO:161[A]:ARG:C | 2.53 | 0.46 |
| 17:OO:28[A]:LEU:CD1 | 17:OO:103[A]:LEU:HB2 | 2.45 | 0.46 |
| 18:PP:158:GLU:HA | 18:PP:159:LYS:HB2 | 1.97 | 0.46 |
| 83:1:388:THR:HG22 | 83:1:395:TYR:CE1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 83:1:491:VAL:HG21 | 83:1:542:LEU:HD11 | 1.97 | 0.46 |
| 83:1:582:LYS:HZ1 | 83:1:694:HIS:CE1 | 2.33 | 0.46 |
| 81:2:1326:C:C4 | 81:2:1327:G:N7 | 2.83 | 0.46 |
| 81:2:1604:C:H2' | 81:2:1605:G:C8 | 2.50 | 0.46 |
| 81:2:487:G:C2 | 81:2:499:C:C2 | 3.03 | 0.46 |
| 81:2:508:G:H2' | 81:2:509:G:C8 | 2.50 | 0.46 |
| 1:5:2438:G:N2 | 1:5:2439:C:C2 | 2.84 | 0.46 |
| 1:5:370:U:C4 | 1:5:371:G:C5 | 3.03 | 0.46 |
| 1:5:436:A:H2' | 1:5:437:G:C8 | 2.50 | 0.46 |
| 1:5:68:C:H2' | 1:5:69:C:O4' | 2.15 | 0.46 |
| 1:5:863:U:H2' | 1:5:864:C:O4' | 2.15 | 0.46 |
| 2:7:88:G:C2 | 2:7:94:C:C2 | 3.03 | 0.46 |
| 6:CC:200:THR:O | 6:CC:201:GLN:HG2 | 2.16 | 0.46 |
| 8:EE:50:VAL:HG13 | 8:EE:51:VAL:N | 2.29 | 0.46 |
| 81:2:1322:C:H6 | 81:2:1322:C:O5' | 1.99 | 0.46 |
| 81:2:1546:G:N2 | 81:2:1547:C:C2 | 2.84 | 0.46 |
| 81:2:609:G:N3 | 81:2:609:G:H2' | 2.29 | 0.46 |
| 1:5:1193:G:H5' | 1:5:1194:A:C2 | 2.51 | 0.46 |
| 1:5:2218:G:O2' | 1:5:2219:G:H8 | 1.98 | 0.46 |
| 1:5:2481:C:C4 | 1:5:2482:U:C4 | 3.04 | 0.46 |
| 1:5:2631:A:H2' | 1:5:2632:C:O4' | 2.15 | 0.46 |
| 1:5:3104:G:C5 | 1:5:3105:C:C5 | 3.03 | 0.46 |
| 1:5:435:C:C2 | 1:5:598:G:N1 | 2.84 | 0.46 |
| 1:5:466:G:C2 | 1:5:467:C:C2 | 3.04 | 0.46 |
| 1:5:78:U:O4 | 1:5:325:A:C2 | 2.61 | 0.46 |
| 1:5:842:U:H2' | 1:5:843:U:O4' | 2.15 | 0.46 |
| 1:5:860:U:H2' | 1:5:861:C:O4' | 2.16 | 0.46 |
| 3:8:56:G:C6 | 3:8:57:C:C4 | 3.03 | 0.46 |
| 5:BB:233:TRP:CD1 | 5:BB:265:ALA:HB1 | 2.51 | 0.46 |
| 5:BB:58:ARG:NH1 | 5:BB:283:TYR:OH | 2.48 | 0.46 |
| 54:G:155:ASP:H | 81:2:78:A:H5'' | 1.73 | 0.46 |
| 11:HH:41:ILE:HD13 | 11:HH:41:ILE:O | 2.15 | 0.46 |
| 57:J:92:LYS:O | 57:J:94:ASP:N | 2.43 | 0.46 |
| 19:QQ:29:LEU:HD21 | 19:QQ:124:LEU:HB2 | 1.97 | 0.46 |
| 19:QQ:44:PHE:CE1 | 19:QQ:139:ILE:HD11 | 2.51 | 0.46 |
| 83:1:388:THR:HG22 | 83:1:395:TYR:CZ | 2.50 | 0.46 |
| 81:2:1154:G:C2 | 81:2:1622:C:C2 | 3.03 | 0.46 |
| 81:2:1641:U:O2 | 81:2:1778:G:N2 | 2.49 | 0.46 |
| 81:2:311:A:N6 | 81:2:351:A:O2' | 2.49 | 0.46 |
| 81:2:407:C:H2' | 81:2:408:C:C6 | 2.51 | 0.46 |
| 82:4:6044:G:C2 | 82:4:6045:C:C2 | 3.03 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:1139:U:H1' | 9:FF:206:ASN:HD22 | 1.81 | 0.46 |
| 1:5:1278:G:C2 | 1:5:1279:A:C2 | 3.04 | 0.46 |
| 1:5:1925:G:N2 | 1:5:2056:C:H2' | 2.20 | 0.46 |
| 1:5:1925:G:O6 | 1:5:2057:A:C6 | 2.67 | 0.46 |
| 1:5:2238:U:O4 | 1:5:2239:A:C5 | 2.67 | 0.46 |
| 1:5:305:U:O2 | 1:5:2752:G:N2 | 2.48 | 0.46 |
| 1:5:314:U:H2' | 1:5:315:C:C6 | 2.51 | 0.46 |
| 1:5:3192:G:N2 | 1:5:3193:C:C2 | 2.83 | 0.46 |
| 1:5:3252:G:O2' | 1:5:3253:C:O4' | 2.24 | 0.46 |
| 1:5:3254:G:C6 | 1:5:3255:C:C4 | 3.04 | 0.46 |
| 5:BB:252:ILE:HG22 | 5:BB:253:GLY:N | 2.30 | 0.46 |
| 8:EE:114:ARG:O | 8:EE:115:ALA:HB3 | 2.14 | 0.46 |
| 9:FF:151:GLY:N | 9:FF:158:ILE:O | 2.42 | 0.46 |
| 17:OO:30[A]:ASN:C | 17:OO:32[A]:GLN:H | 2.18 | 0.46 |
| 70:W:26:LEU:HD11 | 70:W:60:LYS:HD3 | 1.98 | 0.46 |
| 81:2:1290:G:N2 | 81:2:1324:A:N3 | 2.63 | 0.46 |
| 81:2:360:C:N3 | 81:2:383:G:C2 | 2.82 | 0.46 |
| 81:2:407:C:O2' | 81:2:1730:A:O2' | 2.32 | 0.46 |
| 1:5:1111:G:C2 | 1:5:1112:C:C2 | 3.04 | 0.46 |
| 1:5:2507:U:C2' | 1:5:2507:U:O2 | 2.64 | 0.46 |
| 1:5:2540:A:O2' | 1:5:2540:A:N3 | 2.48 | 0.46 |
| 1:5:30:G:C6 | 1:5:31:C:C4 | 3.04 | 0.46 |
| 1:5:701:G:C6 | 1:5:702:C:C4 | 3.04 | 0.46 |
| 2:7:25:G:C2 | 2:7:26:C:C2 | 3.03 | 0.46 |
| 59:L:101:GLU:OE2 | 71:X:13:ARG:N | 2.48 | 0.46 |
| 27:YY:59:VAL:HG13 | 27:YY:60:ARG:HG2 | 1.96 | 0.46 |
| 83:1:154:VAL:HG21 | 83:1:342:LEU:HD11 | 1.97 | 0.46 |
| 83:1:693:LEU:HB3 | 83:1:700:ARG:HH12 | 1.79 | 0.46 |
| 81:2:1588:G:C2 | 81:2:1589:C:C2 | 3.03 | 0.46 |
| 81:2:1651:C:H2' | 81:2:1652:G:O4' | 2.15 | 0.46 |
| 81:2:782:G:N2 | 81:2:783:C:C2 | 2.83 | 0.46 |
| 81:2:85:A:N3 | 81:2:147:U:O2' | 2.49 | 0.46 |
| 81:2:883:A:C2' | 81:2:884:G:H5' | 2.45 | 0.46 |
| 1:5:1769:A:H2' | 1:5:1770:U:O4' | 2.15 | 0.46 |
| 1:5:2264:A:C6 | 24:VV:37:MET:HG3 | 2.51 | 0.46 |
| 1:5:466:G:N2 | 1:5:467:C:C2 | 2.84 | 0.46 |
| 1:5:88:A:H2' | 1:5:89:A:O4' | 2.15 | 0.46 |
| 3:8:118:C:N3 | 3:8:136:G:C2 | 2.84 | 0.46 |
| 48:A:197:ILE:HG23 | 48:A:198:MET:N | 2.30 | 0.46 |
| 1:5:3280:U:H4' | 5:BB:25:VAL:HG21 | 1.98 | 0.46 |
| 14:LL:93:ILE:HG22 | 14:LL:93:ILE:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 83:1:222:ILE:HD11 | 83:1:245:TRP:CE3 | 2.51 | 0.46 |
| 81:2:1120:C:C2 | 81:2:1126:G:C2 | 3.04 | 0.46 |
| 81:2:580:U:O2 | 81:2:580:U:H3' | 2.15 | 0.46 |
| 81:2:935:G:C2 | 81:2:936:C:C2 | 3.04 | 0.46 |
| 1:5:1210:C:C2 | 1:5:1221:G:N1 | 2.84 | 0.46 |
| 1:5:1928:A:C6 | 1:5:2054:U:C2 | 3.04 | 0.46 |
| 1:5:2163:G:N1 | 1:5:2164:C:C4 | 2.84 | 0.46 |
| 1:5:2482:U:O2' | 1:5:2483:U:O5' | 2.33 | 0.46 |
| 1:5:3283:A:H2' | 5:BB:123:TYR:CD2 | 2.51 | 0.46 |
| 5:BB:114:VAL:CG2 | 5:BB:163:HIS:CG | 2.99 | 0.46 |
| 5:BB:256:HIS:HA | 5:BB:257:PRO:C | 2.35 | 0.46 |
| 11:HH:41:ILE:HD11 | 11:HH:67:ALA:HB1 | 1.98 | 0.46 |
| 14:LL:79:GLU:OE2 | 14:LL:103:ASN:ND2 | 2.48 | 0.46 |
| 16:NN:121:ILE:HG22 | 16:NN:122:ASN:HB2 | 1.98 | 0.46 |
| 16:NN:6:TYR:O | 16:NN:10:LEU:N | 2.48 | 0.46 |
| 17:OO:188[A]:THR:O | 17:OO:189[A]:GLU:C | 2.53 | 0.46 |
| 83:1:127:VAL:HG21 | 83:1:143:LEU:HD13 | 1.96 | 0.46 |
| 83:1:211:PHE:HB2 | 83:1:220:PHE:CZ | 2.51 | 0.46 |
| 83:1:698:ILE:CA | 83:1:699:HIS:CB | 2.89 | 0.46 |
| 83:1:79:SER:OG | 83:1:80:GLU:N | 2.49 | 0.46 |
| 81:2:1115:A:C6 | 81:2:1130:A:C8 | 3.04 | 0.46 |
| 81:2:1173:C:C2 | 81:2:1464:G:N2 | 2.84 | 0.46 |
| 81:2:623:G:C6 | 81:2:624:C:C4 | 3.04 | 0.46 |
| 81:2:630:G:C6 | 81:2:631:U:N3 | 2.84 | 0.46 |
| 61:N:114:ARG:NH2 | 81:2:938:A:OP1 | 2.48 | 0.46 |
| 61:N:128:TYR:OH | 81:2:962:A:H4' | 2.16 | 0.46 |
| 1:5:1149:G:N3 | 1:5:1299:C:O2' | 2.49 | 0.46 |
| 1:5:12:A:C2 | 1:5:13:A:C6 | 3.04 | 0.46 |
| 1:5:128:G:N1 | 1:5:141:C:C2 | 2.84 | 0.46 |
| 1:5:1627:G:H2' | 1:5:1628:U:O4' | 2.16 | 0.46 |
| 1:5:2234:C:C3' | 1:5:2235:U:H5' | 2.29 | 0.46 |
| 4:AA:181:LYS:O | 4:AA:182:ALA:C | 2.54 | 0.46 |
| 12:II:51:HIS:ND1 | 12:II:137:SER:OG | 2.44 | 0.46 |
| 1:5:638:A:OP1 | 16:NN:203:ARG:NH1 | 2.48 | 0.46 |
| 17:OO:126[A]:ARG:HG2 | 17:OO:130[A]:LEU:HB2 | 1.97 | 0.46 |
| 17:OO:192[A]:GLU:O | 17:OO:194[A]:LEU:C | 2.54 | 0.46 |
| 24:VV:79:VAL:HG12 | 24:VV:122:CYS:SG | 2.56 | 0.46 |
| 81:2:925:A:H3' | 81:2:926:C:C6 | 2.51 | 0.46 |
| 1:5:1288:A:H5' | 1:5:1288:A:N3 | 2.31 | 0.46 |
| 1:5:1335:C:O2' | 1:5:1336:G:H5' | 2.16 | 0.46 |
| 1:5:2630:G:H2' | 1:5:2631:A:H8 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 1:5:2886:G:N2 | 1:5:2897:C:C2 | 2.84 | 0.46 |
| 1:5:2922:U:O4' | 1:5:2922:U:O2 | 2.32 | 0.46 |
| 5:BB:114:VAL:O | 5:BB:117:ARG:N | 2.45 | 0.46 |
| 12:II:36:LEU:HD21 | 12:II:69:ARG:HD3 | 1.97 | 0.46 |
| 57:J:140:ILE:HD12 | 72:Y:65:GLY:HA3 | 1.98 | 0.46 |
| 17:OO:113[A]:TYR:C | 17:OO:115[A]:LYS:N | 2.68 | 0.46 |
| 17:OO:122[A]:PRO:HA | 17:OO:125[A]:LEU:HD22 | 1.94 | 0.46 |
| 17:OO:162[A]:LYS:O | 17:OO:166[A]:ALA:N | 2.45 | 0.46 |
| 83:1:589:LYS:CD | 83:1:685:ARG:CD | 2.89 | 0.46 |
| 81:2:1328:A:H2' | 81:2:1329:G:O4' | 2.16 | 0.46 |
| 81:2:1482:G:N2 | 81:2:1483:C:C2 | 2.84 | 0.46 |
| 81:2:1661:G:C2 | 81:2:1662:C:C2 | 3.03 | 0.46 |
| 81:2:23:G:O2' | 81:2:24:U:C5' | 2.64 | 0.46 |
| 81:2:991:A:N3 | 81:2:991:A:C5' | 2.79 | 0.46 |
| 1:5:1314:A:C2 | 1:5:1333:G:C2 | 3.04 | 0.46 |
| 1:5:2218:G:C2' | 1:5:2219:G:C5' | 2.94 | 0.46 |
| 1:5:3174:C:N3 | 15:MM:13:ARG:NH2 | 2.63 | 0.46 |
| 1:5:340:C:N3 | 3:8:25:G:C2 | 2.84 | 0.46 |
| 3:8:75:G:C6 | 3:8:76:C:C4 | 3.04 | 0.46 |
| 6:CC:74:ILE:HD11 | 6:CC:93:MET:HE2 | 1.97 | 0.46 |
| 17:OO:113[A]:TYR:O | 17:OO:115[A]:LYS:N | 2.49 | 0.46 |
| 17:OO:11[A]:ASP:HB2 | 17:OO:118[A]:ARG:HG3 | 1.98 | 0.46 |
| 17:OO:29[A]:LEU:HB3 | 17:OO:95[A]:ARG:NH2 | 2.30 | 0.46 |
| 65:R:7:LYS:O | 65:R:11:ARG:N | 2.46 | 0.46 |
| 83:1:118:ALA:O | 83:1:122:THR:HG23 | 2.17 | 0.45 |
| 81:2:301:U:O2 | 81:2:301:U:H2' | 2.15 | 0.45 |
| 1:5:1120:G:C2 | 1:5:1126:C:C2 | 3.04 | 0.45 |
| 1:5:1587:G:C2 | 1:5:1796:C:C2 | 3.05 | 0.45 |
| 1:5:1637:G:C2 | 1:5:1638:C:C2 | 3.03 | 0.45 |
| 1:5:1690:U:O4 | 20:RR:128:LYS:NZ | 2.42 | 0.45 |
| 1:5:1874:G:O6 | 5:BB:241:LYS:NZ | 2.37 | 0.45 |
| 1:5:2541:C:C4 | 1:5:2542:G:C8 | 3.04 | 0.45 |
| 1:5:2711:A:H2' | 1:5:2712:U:O4' | 2.16 | 0.45 |
| 1:5:3161:C:C2 | 1:5:3168:G:C2 | 3.04 | 0.45 |
| 21:SS:87:THR:HG23 | 22:TT:156:TYR:CG | 2.51 | 0.45 |
| 83:1:20:ARG:CZ | 83:1:342:LEU:HD13 | 2.47 | 0.45 |
| 83:1:657:HIS:HA | 83:1:660:LYS:HD2 | 1.96 | 0.45 |
| 81:2:1298:G:C2 | 81:2:1299:A:C2 | 3.04 | 0.45 |
| 81:2:1647:G:H2' | 81:2:1648:U:C6 | 2.51 | 0.45 |
| 57:J:170:GLY:CA | 81:2:510:A:C3' | 2.94 | 0.45 |
| 81:2:882:C:C2 | 81:2:883:A:C8 | 3.04 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 81:2:991:A:N3 | 81:2:991:A:H5' | 2.32 | 0.45 |
| 1:5:1328:G:C5 | 1:5:1329:C:C4 | 3.04 | 0.45 |
| 1:5:1729:C:N3 | 1:5:1735:G:C6 | 2.84 | 0.45 |
| 1:5:16:A:H2' | 1:5:17:G:O4' | 2.16 | 0.45 |
| 1:5:1087:G:N2 | 1:5:2785:A:O4' | 2.49 | 0.45 |
| 1:5:590:G:C2 | 1:5:591:C:C2 | 3.04 | 0.45 |
| 1:5:954:A:H3' | 1:5:955:G:C5' | 2.46 | 0.45 |
| 3:8:140:G:C6 | 3:8:141:C:N3 | 2.85 | 0.45 |
| 1:5:211:A:OP1 | 6:CC:220:ARG:HD2 | 2.16 | 0.45 |
| 6:CC:65:TRP:CD1 | 6:CC:69:ARG:HD2 | 2.52 | 0.45 |
| 58:K:55:VAL:CG2 | 58:K:68:LEU:HD23 | 2.47 | 0.45 |
| 17:OO:106[A]:PHE:CD2 | 17:OO:110[A]:PRO:HG3 | 2.51 | 0.45 |
| 18:PP:41:LEU:HD21 | 18:PP:95:LEU:HB3 | 1.97 | 0.45 |
| 81:2:108:A:H2' | 81:2:109:G:C8 | 2.51 | 0.45 |
| 81:2:1290:G:C2 | 81:2:1324:A:C2 | 3.04 | 0.45 |
| 81:2:1502:G:N7 | 81:2:1503:A:C2 | 2.84 | 0.45 |
| 81:2:281:C:H2' | 81:2:282:U:O4' | 2.16 | 0.45 |
| 81:2:48:G:C6 | 81:2:49:C:C4 | 3.05 | 0.45 |
| 81:2:561:G:C2 | 81:2:583:C:C2 | 3.05 | 0.45 |
| 1:5:1145:G:C6 | 1:5:1146:C:C4 | 3.05 | 0.45 |
| 1:5:1637:G:C6 | 1:5:1638:C:C4 | 3.04 | 0.45 |
| 1:5:2235:U:O2' | 1:5:2236:C:C6 | 2.68 | 0.45 |
| 1:5:2983:G:C2 | 1:5:3008:A:C2 | 3.05 | 0.45 |
| 1:5:3120:U:H4' | 1:5:3121:U:OP2 | 2.16 | 0.45 |
| 1:5:830:G:C2 | 1:5:832:C:C2 | 3.05 | 0.45 |
| 3:8:114:G:N2 | 3:8:115:C:C2 | 2.84 | 0.45 |
| 7:DD:49:TYR:CE1 | 7:DD:66:SER:HB2 | 2.51 | 0.45 |
| 57:J:76:LEU:HD21 | 57:J:96:VAL:HG11 | 1.98 | 0.45 |
| 16:NN:16:SER:OG | 16:NN:19:LEU:HB2 | 2.16 | 0.45 |
| 18:PP:33:ALA:HB1 | 18:PP:117:ILE:HG12 | 1.99 | 0.45 |
| 19:QQ:182:ARG:O | 19:QQ:183:ALA:HB3 | 2.16 | 0.45 |
| 65:R:25:THR:O | 65:R:27:ASP:N | 2.49 | 0.45 |
| 81:2:430:C:H4' | 83:1:392:GLY:HA3 | 1.97 | 0.45 |
| 83:1:49:ALA:HB1 | 83:1:50:LYS:HA | 1.99 | 0.45 |
| 81:2:1171:G:C2 | 81:2:1172:C:C2 | 3.05 | 0.45 |
| 81:2:1307:G:C2 | 81:2:1308:C:C2 | 3.05 | 0.45 |
| 81:2:360:C:C2 | 81:2:383:G:C2 | 3.04 | 0.45 |
| 81:2:878:G:C2 | 81:2:879:C:C2 | 3.05 | 0.45 |
| 1:5:1589:U:H2' | 1:5:1590:A:C8 | 2.52 | 0.45 |
| 1:5:2244:A:N6 | 1:5:2280:G:H1' | 2.32 | 0.45 |
| 1:5:2414:A:H3' | 1:5:2415:U:O4' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|----------------------|--------------------------|-------------------|
| 1:5:2480:A:C8 | 1:5:2481:C:C6 | 3.04 | 0.45 |
| 2:7:43:U:C4 | 2:7:44:C:C4 | 3.04 | 0.45 |
| 4:AA:209:HIS:CD2 | 4:AA:209:HIS:C | 2.90 | 0.45 |
| 54:G:154:ARG:N | 81:2:78:A:C5' | 2.77 | 0.45 |
| 19:QQ:71:LEU:CD1 | 19:QQ:99:THR:HG21 | 2.46 | 0.45 |
| 24:VV:17:LEU:HB2 | 24:VV:52:ALA:HB3 | 1.97 | 0.45 |
| 70:W:11:LEU:HD12 | 70:W:74:VAL:CG2 | 2.46 | 0.45 |
| 28:ZZ:15:ARG:HD3 | 28:ZZ:79:HIS:CD2 | 2.51 | 0.45 |
| 83:1:559:PRO:HB2 | 83:1:561:VAL:HG13 | 1.99 | 0.45 |
| 83:1:685:ARG:NH1 | 83:1:685:ARG:CG | 2.73 | 0.45 |
| 82:4:6136:U:H2' | 82:4:6137:A:O4' | 2.17 | 0.45 |
| 1:5:1194:A:C4 | 1:5:1195:C:C6 | 3.04 | 0.45 |
| 1:5:167:U:H2' | 1:5:168:U:O4' | 2.16 | 0.45 |
| 1:5:2606:C:O2 | 22:TT:60:LYS:NZ | 2.49 | 0.45 |
| 1:5:2620:U:C4 | 1:5:2621:C:C4 | 3.04 | 0.45 |
| 1:5:77:A:OP2 | 14:LL:73:ARG:NH2 | 2.50 | 0.45 |
| 4:AA:112:ILE:HG23 | 4:AA:133:TYR:CD2 | 2.51 | 0.45 |
| 50:C:145:ARG:HG3 | 50:C:227:TYR:CE1 | 2.52 | 0.45 |
| 6:CC:295:ILE:HG22 | 6:CC:299:LEU:HD11 | 1.98 | 0.45 |
| 17:OO:130[A]:LEU:HD12 | 17:OO:130[A]:LEU:HA | 1.60 | 0.45 |
| 11:HH:4:ILE:N | 21:SS:142:GLN:OE1 | 2.48 | 0.45 |
| 83:1:488:VAL:HG13 | 83:1:489:VAL:N | 2.32 | 0.45 |
| 81:2:1021:C:O2' | 81:2:1124:A:N1 | 2.47 | 0.45 |
| 81:2:1438:C:H2' | 81:2:1439:C:O5' | 2.16 | 0.45 |
| 81:2:1440:U:O4 | 81:2:1441:U:O4 | 2.34 | 0.45 |
| 81:2:66:U:O4' | 81:2:66:U:O2 | 2.34 | 0.45 |
| 81:2:878:G:C6 | 81:2:879:C:C4 | 3.05 | 0.45 |
| 81:2:887:U:C4 | 81:2:888:U:C4 | 3.05 | 0.45 |
| 82:4:6120:U:H1' | 82:4:6127:C:C3' | 2.46 | 0.45 |
| 1:5:1670:C:H2' | 1:5:1671:U:O4' | 2.16 | 0.45 |
| 1:5:2268:A:C5 | 1:5:2269:G:C8 | 3.05 | 0.45 |
| 1:5:2482:U:C4 | 1:5:2560:G:C4 | 3.05 | 0.45 |
| 1:5:2482:U:C5 | 1:5:2560:G:C5 | 3.04 | 0.45 |
| 1:5:967:A:C2 | 1:5:1025:A:C4 | 3.05 | 0.45 |
| 5:BB:229:VAL:HG22 | 5:BB:266:ARG:HA | 1.99 | 0.45 |
| 5:BB:73:VAL:HG21 | 25:WW:16:GLY:CA | 2.47 | 0.45 |
| 7:DD:83:LEU:N | 7:DD:84:PRO:HD2 | 2.32 | 0.45 |
| 54:G:136:LYS:HZ3 | 54:G:176:GLN:HB2 | 1.82 | 0.45 |
| 16:NN:60:VAL:HG12 | 16:NN:61:ILE:N | 2.32 | 0.45 |
| 17:OO:16[A]:LEU:HA | 17:OO:16[A]:LEU:HD23 | 1.71 | 0.45 |
| 17:OO:176[A]:ASN:C | 17:OO:178[A]:VAL:H | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:5:1691:U:OP1 | 20:RR:100:ARG:NH1 | 2.49 | 0.45 |
| 83:1:519:LEU:CD1 | 83:1:521:TYR:HB3 | 2.46 | 0.45 |
| 83:1:694:HIS:N | 83:1:695:ALA:HA | 2.31 | 0.45 |
| 81:2:1126:G:C2 | 81:2:1127:C:C2 | 3.05 | 0.45 |
| 82:4:6119:U:OP1 | 82:4:6120:U:C2 | 2.70 | 0.45 |
| 1:5:1664:U:C2 | 1:5:1718:A:C2 | 3.04 | 0.45 |
| 1:5:1722:G:H2' | 1:5:1723:C:O4' | 2.16 | 0.45 |
| 1:5:2220:G:H2' | 1:5:2221:A:O4' | 2.17 | 0.45 |
| 1:5:2491:U:O2 | 1:5:2491:U:O4' | 2.32 | 0.45 |
| 1:5:385:A:H2' | 1:5:386:A:C8 | 2.52 | 0.45 |
| 1:5:595:A:C5 | 1:5:596:U:C5 | 3.04 | 0.45 |
| 3:8:49:G:C2 | 3:8:50:C:C2 | 3.05 | 0.45 |
| 4:AA:182:ALA:O | 4:AA:185:ALA:N | 2.49 | 0.45 |
| 59:L:132:SER:O | 59:L:133:LYS:C | 2.55 | 0.45 |
| 81:2:10:G:H2' | 81:2:11:A:H8 | 1.81 | 0.45 |
| 81:2:1598:A:H1' | 81:2:1599:G:C5' | 2.46 | 0.45 |
| 81:2:562:U:H3' | 81:2:563:G:C8 | 2.52 | 0.45 |
| 81:2:903:G:O2' | 81:2:904:A:N7 | 2.50 | 0.45 |
| 81:2:988:U:C4 | 81:2:989:C:N4 | 2.85 | 0.45 |
| 1:5:1926:U:N3 | 1:5:1927:G:C8 | 2.84 | 0.45 |
| 1:5:1926:U:C2 | 1:5:1927:G:C8 | 3.05 | 0.45 |
| 1:5:2237:U:C6 | 1:5:2239:A:OP2 | 2.70 | 0.45 |
| 1:5:2479:U:O2' | 1:5:2480:A:C5' | 2.59 | 0.45 |
| 1:5:2479:U:N3 | 1:5:2480:A:N7 | 2.65 | 0.45 |
| 1:5:2480:A:N7 | 1:5:2481:C:C6 | 2.84 | 0.45 |
| 1:5:3055:A:C5' | 1:5:3055:A:C8 | 2.99 | 0.45 |
| 1:5:3205:U:H2' | 1:5:3206:A:O4' | 2.17 | 0.45 |
| 1:5:3232:G:C6 | 1:5:3233:C:C4 | 3.04 | 0.45 |
| 1:5:601:A:C2 | 1:5:602:A:C4 | 3.05 | 0.45 |
| 1:5:675:C:O2 | 1:5:759:C:H4' | 2.17 | 0.45 |
| 1:5:886:A:H2' | 1:5:886:A:N3 | 2.32 | 0.45 |
| 1:5:780:G:N1 | 1:5:903:U:O4 | 2.49 | 0.45 |
| 4:AA:113:ILE:HD12 | 4:AA:136:VAL:HG23 | 1.99 | 0.45 |
| 6:CC:338:LYS:O | 6:CC:340:GLY:N | 2.50 | 0.45 |
| 1:5:75:G:H5' | 14:LL:58:VAL:HG13 | 1.98 | 0.45 |
| 17:OO:118[A]:ARG:C | 17:OO:119[A]:VAL:CG1 | 2.85 | 0.45 |
| 17:OO:184[A]:ALA:C | 17:OO:186[A]:VAL:N | 2.70 | 0.45 |
| 21:SS:132:THR:O | 21:SS:133:ALA:CB | 2.64 | 0.45 |
| 22:TT:62:GLY:HA3 | 22:TT:76:ILE:HD13 | 1.99 | 0.45 |
| 5:BB:73:VAL:HG21 | 25:WW:16:GLY:HA3 | 1.99 | 0.45 |
| 26:XX:67:ILE:HD12 | 26:XX:83:VAL:HG12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 83:1:694:HIS:H | 83:1:695:ALA:HA | 1.81 | 0.45 |
| 81:2:268:G:C2 | 81:2:269:C:C2 | 3.05 | 0.45 |
| 81:2:935:G:N2 | 81:2:936:C:C2 | 2.85 | 0.45 |
| 82:4:6121:A:C4 | 82:4:6121:A:OP2 | 2.70 | 0.45 |
| 1:5:1339:U:O2' | 1:5:1340:A:H5' | 2.16 | 0.45 |
| 1:5:1873:C:H2' | 1:5:1874:G:O4' | 2.17 | 0.45 |
| 1:5:2287:U:H2' | 1:5:2288:U:O4' | 2.17 | 0.45 |
| 1:5:2302:C:H2' | 1:5:2303:U:O4' | 2.16 | 0.45 |
| 1:5:964:G:N3 | 1:5:2605:A:H2' | 2.32 | 0.45 |
| 1:5:2852:C:N3 | 1:5:2907:G:C6 | 2.85 | 0.45 |
| 1:5:3054:A:H3' | 1:5:3055:A:C8 | 2.51 | 0.45 |
| 1:5:308:A:C6 | 1:5:309:U:C4 | 3.04 | 0.45 |
| 1:5:987:C:C2' | 1:5:987:C:O2 | 2.65 | 0.45 |
| 4:AA:32:LEU:HD22 | 4:AA:163:ARG:CZ | 2.47 | 0.45 |
| 5:BB:218:VAL:HA | 5:BB:276:THR:HA | 1.99 | 0.45 |
| 6:CC:169:LEU:HB3 | 6:CC:174:ALA:HB3 | 1.99 | 0.45 |
| 7:DD:39:GLN:HE21 | 7:DD:43:LYS:HD2 | 1.81 | 0.45 |
| 8:EE:112:LYS:HD2 | 8:EE:113:GLN:H | 1.82 | 0.45 |
| 55:H:118:LEU:HB3 | 81:2:638:U:OP2 | 2.16 | 0.45 |
| 55:H:98:ILE:HG12 | 55:H:121:VAL:HG21 | 1.99 | 0.45 |
| 59:L:113:PRO:O | 59:L:116:ARG:NH2 | 2.47 | 0.45 |
| 59:L:74:THR:HA | 59:L:122:ILE:HA | 1.99 | 0.45 |
| 59:L:66:ILE:HG13 | 59:L:140:LEU:HD21 | 1.99 | 0.45 |
| 62:O:134:GLY:O | 62:O:136:ARG:HG3 | 2.17 | 0.45 |
| 61:N:18:TYR:O | 70:W:56:HIS:CG | 2.70 | 0.45 |
| 81:2:1586:G:N2 | 81:2:1587:C:H1' | 2.31 | 0.45 |
| 81:2:311:A:N7 | 81:2:351:A:C2 | 2.85 | 0.45 |
| 81:2:362:G:N2 | 81:2:381:C:C2 | 2.84 | 0.45 |
| 81:2:452:U:C2' | 81:2:452:U:O2 | 2.65 | 0.45 |
| 1:5:2238:U:C4 | 1:5:2239:A:C8 | 3.05 | 0.45 |
| 1:5:2970:C:H2' | 1:5:2971:G:O4' | 2.17 | 0.45 |
| 1:5:3007:C:H2' | 1:5:3008:A:O4' | 2.17 | 0.45 |
| 1:5:504:A:C6 | 1:5:529:U:C5 | 3.04 | 0.45 |
| 3:8:119:C:C2 | 3:8:135:G:N2 | 2.85 | 0.45 |
| 1:5:845:U:OP1 | 5:BB:241:LYS:HG3 | 2.17 | 0.45 |
| 8:EE:151:THR:CG2 | 8:EE:154:LEU:HD12 | 2.47 | 0.45 |
| 12:II:69:ARG:HD2 | 12:II:69:ARG:C | 2.37 | 0.45 |
| 61:N:115:LEU:HD22 | 61:N:115:LEU:O | 2.17 | 0.45 |
| 17:OO:5[A]:GLU:HB3 | 17:OO:6[A]:PRO:HD2 | 1.98 | 0.45 |
| 69:V:33:GLN:HE21 | 69:V:33:GLN:HA | 1.82 | 0.45 |
| 73:Z:74:SER:HB2 | 81:2:1531:C:OP2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 83:1:245:TRP:O | 83:1:245:TRP:CD1 | 2.70 | 0.44 |
| 81:2:1032:C:N4 | 81:2:1033:C:N4 | 2.64 | 0.44 |
| 81:2:1093:G:C2' | 81:2:1094:U:O5' | 2.65 | 0.44 |
| 81:2:1580:U:O2 | 81:2:1611:U:H5 | 2.00 | 0.44 |
| 81:2:1620:G:C6 | 81:2:1621:C:C4 | 3.04 | 0.44 |
| 81:2:811:A:H4' | 81:2:812:U:O5' | 2.16 | 0.44 |
| 1:5:1356:C:C2 | 1:5:1393:G:N1 | 2.85 | 0.44 |
| 1:5:2132:C:OP1 | 4:AA:231:SER:HA | 2.17 | 0.44 |
| 1:5:247:A:C4 | 1:5:248:U:H1' | 2.52 | 0.44 |
| 1:5:2574:G:N3 | 1:5:2574:G:H2' | 2.31 | 0.44 |
| 1:5:262:U:H2' | 1:5:263:C:O4' | 2.17 | 0.44 |
| 1:5:3359:A:H2' | 1:5:3360:U:O4' | 2.17 | 0.44 |
| 1:5:601:A:C2 | 1:5:602:A:C2 | 3.06 | 0.44 |
| 1:5:770:G:O2' | 14:LL:18:TRP:NE1 | 2.41 | 0.44 |
| 17:OO:6[A]:PRO:HB2 | 17:OO:7[A]:VAL:H | 1.53 | 0.44 |
| 71:X:86:PHE:CD1 | 71:X:117:ILE:HD13 | 2.51 | 0.44 |
| 26:XX:115:ARG:NH1 | 26:XX:119:THR:OG1 | 2.50 | 0.44 |
| 83:1:25:ILE:HG12 | 83:1:119:LEU:HD11 | 1.99 | 0.44 |
| 83:1:562:ALA:HB1 | 83:1:563:TYR:CA | 2.32 | 0.44 |
| 83:1:573:GLN:HA | 83:1:574:THR:HG23 | 1.99 | 0.44 |
| 81:2:1590:A:C2 | 81:2:1591:A:C6 | 3.06 | 0.44 |
| 57:J:170:GLY:CA | 81:2:511:A:O4' | 2.65 | 0.44 |
| 1:5:1356:C:O2 | 1:5:1393:G:C2 | 2.71 | 0.44 |
| 1:5:2671:A:C6 | 7:DD:150:LEU:HD11 | 2.53 | 0.44 |
| 1:5:30:G:C2 | 1:5:31:C:C2 | 3.06 | 0.44 |
| 1:5:3208:C:H2' | 1:5:3209:G:O4' | 2.17 | 0.44 |
| 2:7:112:G:C2 | 2:7:113:C:C2 | 3.05 | 0.44 |
| 4:AA:107:VAL:HG12 | 4:AA:111:THR:OG1 | 2.17 | 0.44 |
| 5:BB:86:VAL:HG13 | 5:BB:160:VAL:CG1 | 2.46 | 0.44 |
| 9:FF:218:LYS:O | 9:FF:219:HIS:CB | 2.65 | 0.44 |
| 54:G:4:ASN:HB3 | 54:G:110:ALA:HA | 1.99 | 0.44 |
| 11:HH:18:VAL:HG12 | 11:HH:27:VAL:HG13 | 1.99 | 0.44 |
| 57:J:83:ILE:HG23 | 57:J:85:VAL:HG23 | 1.99 | 0.44 |
| 59:L:152:GLN:HB3 | 59:L:153:PHE:HA | 1.99 | 0.44 |
| 65:R:80:ARG:O | 65:R:84:TYR:N | 2.49 | 0.44 |
| 70:W:11:LEU:HD13 | 70:W:72:CYS:SG | 2.57 | 0.44 |
| 83:1:378:LEU:HG | 83:1:403:GLY:HA3 | 1.97 | 0.44 |
| 81:2:1171:G:C6 | 81:2:1172:C:C4 | 3.06 | 0.44 |
| 81:2:1389:A:H2' | 81:2:1390:U:C6 | 2.53 | 0.44 |
| 81:2:1648:U:H3' | 81:2:1649:A:H8 | 1.82 | 0.44 |
| 81:2:585:G:C2 | 81:2:586:C:C2 | 3.05 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 81:2:604:A:C4 | 81:2:605:A:C2 | 3.06 | 0.44 |
| 81:2:782:G:C6 | 81:2:783:C:C4 | 3.05 | 0.44 |
| 81:2:782:G:C2 | 81:2:783:C:C2 | 3.05 | 0.44 |
| 1:5:1086:G:H5'' | 1:5:1087:G:H5' | 2.00 | 0.44 |
| 1:5:1157:G:C6 | 1:5:1158:C:C4 | 3.06 | 0.44 |
| 1:5:1210:C:C2 | 1:5:1221:G:C2 | 3.06 | 0.44 |
| 1:5:2218:G:C3' | 1:5:2218:G:P | 3.06 | 0.44 |
| 1:5:2285:G:O2' | 1:5:2286:A:O5' | 2.35 | 0.44 |
| 1:5:3291:A:H2' | 1:5:3292:C:O4' | 2.18 | 0.44 |
| 1:5:470:G:C2 | 1:5:471:C:C2 | 3.05 | 0.44 |
| 2:7:10:C:C4 | 7:DD:20:PHE:CD1 | 3.06 | 0.44 |
| 7:DD:20:PHE:O | 7:DD:24:ARG:NH2 | 2.50 | 0.44 |
| 1:5:1097:G:OP2 | 12:II:14:ASN:ND2 | 2.50 | 0.44 |
| 13:JJ:30:LEU:HD23 | 13:JJ:65:ILE:O | 2.18 | 0.44 |
| 17:OO:136[A]:TYR:N | 17:OO:136[A]:TYR:CD1 | 2.85 | 0.44 |
| 17:OO:174[A]:ALA:O | 17:OO:175[A]:TYR:C | 2.55 | 0.44 |
| 63:P:19:GLY:H | 66:S:93:ASN:N | 2.15 | 0.44 |
| 23:UU:80:THR:HG21 | 23:UU:95:PHE:CD1 | 2.52 | 0.44 |
| 83:1:108:HIS:N | 83:1:138:GLN:OE1 | 2.49 | 0.44 |
| 83:1:383:SER:C | 83:1:465:LYS:O | 2.54 | 0.44 |
| 83:1:33:SER:HB3 | 83:1:57:THR:HG21 | 2.00 | 0.44 |
| 83:1:704:GLN:O | 83:1:708:THR:HG22 | 2.18 | 0.44 |
| 81:2:1624:U:H2' | 81:2:1625:U:C6 | 2.51 | 0.44 |
| 81:2:885:U:O2' | 81:2:886:A:H5'' | 2.13 | 0.44 |
| 82:4:6118:U:H2' | 82:4:6119:U:C4' | 2.47 | 0.44 |
| 1:5:1145:G:C2' | 1:5:1146:C:O5' | 2.65 | 0.44 |
| 1:5:1418:G:OP1 | 18:PP:65:SER:OG | 2.29 | 0.44 |
| 1:5:1621:G:H2' | 1:5:1622:G:O4' | 2.17 | 0.44 |
| 1:5:208:C:H2' | 1:5:209:A:O4' | 2.17 | 0.44 |
| 1:5:2163:G:C6 | 1:5:2164:C:N4 | 2.85 | 0.44 |
| 1:5:2244:A:H2' | 1:5:2245:G:O4' | 2.18 | 0.44 |
| 1:5:2804:C:H4' | 12:II:157:TYR:CD2 | 2.52 | 0.44 |
| 1:5:2899:C:H2' | 1:5:2900:U:O4' | 2.17 | 0.44 |
| 1:5:3196:C:H4' | 1:5:3197:G:O5' | 2.17 | 0.44 |
| 1:5:529:U:O4' | 1:5:530:A:C5 | 2.71 | 0.44 |
| 3:8:116:G:C6 | 3:8:117:C:N4 | 2.86 | 0.44 |
| 3:8:49:G:C6 | 3:8:50:C:C4 | 3.05 | 0.44 |
| 5:BB:118:PHE:CE2 | 5:BB:130:PHE:HE1 | 2.36 | 0.44 |
| 5:BB:218:VAL:HG22 | 5:BB:276:THR:HG22 | 1.99 | 0.44 |
| 14:LL:3:ILE:HG13 | 14:LL:4:SER:N | 2.25 | 0.44 |
| 17:OO:152[A]:ASP:OD1 | 17:OO:152[A]:ASP:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|----------------------|--------------------------|-------------------|
| 72:Y:59:GLY:N | 81:2:522:G:OP1 | 2.50 | 0.44 |
| 83:1:276:PHE:CD1 | 83:1:276:PHE:C | 2.90 | 0.44 |
| 83:1:647:ILE:HD12 | 83:1:685:ARG:NH1 | 2.32 | 0.44 |
| 81:2:1671:G:C4 | 81:2:1672:C:C5 | 3.05 | 0.44 |
| 81:2:776:G:N1 | 81:2:777:C:C4 | 2.85 | 0.44 |
| 81:2:922:A:H2' | 81:2:923:A:O4' | 2.18 | 0.44 |
| 81:2:95:G:O2' | 81:2:459:A:O2' | 2.16 | 0.44 |
| 82:4:6198:A:C2 | 82:4:6199:A:C5 | 3.05 | 0.44 |
| 1:5:1193:G:C6 | 1:5:1257:A:O4' | 2.70 | 0.44 |
| 1:5:1266:G:C5 | 1:5:1267:C:C4 | 3.05 | 0.44 |
| 1:5:248:U:C3' | 1:5:249:U:H5' | 2.47 | 0.44 |
| 1:5:269:G:H5' | 16:NN:120:TRP:CE3 | 2.53 | 0.44 |
| 1:5:2799:G:C2 | 1:5:2800:C:C2 | 3.06 | 0.44 |
| 1:5:287:G:C6 | 1:5:288:C:C4 | 3.05 | 0.44 |
| 1:5:63:A:H2 | 1:5:78:U:O2 | 2.01 | 0.44 |
| 4:AA:9:ARG:O | 4:AA:10:LYS:C | 2.56 | 0.44 |
| 7:DD:160:PHE:HA | 7:DD:163:LEU:HB3 | 2.00 | 0.44 |
| 7:DD:178:ASN:HA | 7:DD:183:TRP:CD2 | 2.53 | 0.44 |
| 59:L:20:PHE:CE2 | 59:L:22:ASN:HA | 2.52 | 0.44 |
| 14:LL:47:ALA:HB3 | 14:LL:48:PRO:CD | 2.48 | 0.44 |
| 17:OO:121[A]:VAL:HG12 | 17:OO:123[A]:GLN:HG2 | 1.99 | 0.44 |
| 17:OO:124[A]:ALA:C | 17:OO:125[A]:LEU:O | 2.49 | 0.44 |
| 18:PP:30:ARG:HA | 18:PP:119:VAL:HG11 | 2.00 | 0.44 |
| 20:RR:93:VAL:O | 20:RR:94:VAL:C | 2.56 | 0.44 |
| 22:TT:91:LEU:HD12 | 22:TT:96:ILE:HD11 | 1.99 | 0.44 |
| 71:X:19:ARG:HD2 | 71:X:19:ARG:HA | 1.70 | 0.44 |
| 83:1:491:VAL:HG22 | 83:1:538:LEU:HD21 | 1.99 | 0.44 |
| 81:2:268:G:C6 | 81:2:269:C:C4 | 3.05 | 0.44 |
| 81:2:372:G:N2 | 81:2:602:U:O3' | 2.51 | 0.44 |
| 57:J:170:GLY:HA2 | 81:2:511:A:O4' | 2.10 | 0.44 |
| 81:2:930:C:H5'' | 81:2:931:U:H3' | 1.99 | 0.44 |
| 81:2:963:U:H1' | 81:2:964:U:OP2 | 2.16 | 0.44 |
| 82:4:6182:A:N6 | 82:4:6195:G:O2' | 2.50 | 0.44 |
| 1:5:1193:G:H2' | 1:5:1194:A:C4 | 2.52 | 0.44 |
| 1:5:1633:G:C2 | 1:5:1634:C:C2 | 3.06 | 0.44 |
| 1:5:1825:C:C4 | 1:5:1826:C:N4 | 2.86 | 0.44 |
| 1:5:184:U:H2' | 1:5:185:C:C6 | 2.53 | 0.44 |
| 1:5:2137:A:N6 | 1:5:2139:U:O2 | 2.51 | 0.44 |
| 1:5:2216:G:N3 | 1:5:2240:A:H2 | 2.15 | 0.44 |
| 1:5:2247:C:C2 | 1:5:2276:G:C2 | 3.06 | 0.44 |
| 1:5:172:A:C4 | 1:5:247:A:N6 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:2540:A:C2 | 1:5:2541:C:C4 | 3.06 | 0.44 |
| 1:5:2748:A:H2' | 1:5:2749:U:H5' | 2.00 | 0.44 |
| 1:5:3302:U:H4' | 1:5:3303:A:H5'' | 2.00 | 0.44 |
| 1:5:373:A:C6 | 1:5:375:A:C6 | 3.06 | 0.44 |
| 3:8:145:U:H2' | 3:8:146:U:O4' | 2.17 | 0.44 |
| 3:8:78:G:H2' | 3:8:79:A:O4' | 2.17 | 0.44 |
| 4:AA:183:GLY:O | 4:AA:186:PHE:HB3 | 2.18 | 0.44 |
| 4:AA:6:ARG:CZ | 4:AA:7:ASN:HD21 | 2.30 | 0.44 |
| 9:FF:135:TYR:HE2 | 9:FF:230:GLU:CD | 2.21 | 0.44 |
| 56:I:175:GLY:HA3 | 81:2:330:A:OP1 | 2.18 | 0.44 |
| 57:J:117:GLY:O | 57:J:119:ALA:N | 2.50 | 0.44 |
| 17:OO:171[A]:LYS:NZ | 17:OO:171[A]:LYS:CB | 2.72 | 0.44 |
| 17:OO:42[A]:LEU:HA | 17:OO:42[A]:LEU:HD12 | 1.48 | 0.44 |
| 17:OO:5[A]:GLU:HB3 | 17:OO:6[A]:PRO:CD | 2.46 | 0.44 |
| 21:SS:87:THR:HG23 | 22:TT:156:TYR:CD2 | 2.53 | 0.44 |
| 67:T:61:VAL:HG21 | 67:T:104:VAL:HG11 | 2.00 | 0.44 |
| 70:W:75:ILE:HD11 | 70:W:125:ILE:HB | 1.99 | 0.44 |
| 81:2:1314:U:H2' | 81:2:1315:G:O4' | 2.18 | 0.44 |
| 81:2:1400:G:C2 | 81:2:1401:C:C2 | 3.05 | 0.44 |
| 81:2:1400:G:C6 | 81:2:1401:C:C4 | 3.05 | 0.44 |
| 81:2:1497:G:C2 | 81:2:1498:C:C2 | 3.06 | 0.44 |
| 81:2:1603:G:C2 | 81:2:1604:C:C2 | 3.06 | 0.44 |
| 1:5:916:C:C2 | 1:5:1346:G:C2 | 3.06 | 0.44 |
| 1:5:1397:C:C4 | 1:5:1398:U:C5 | 3.06 | 0.44 |
| 1:5:2282:A:O4' | 1:5:2284:G:C8 | 2.71 | 0.44 |
| 10:GG:32:ASN:O | 10:GG:38:ALA:HB3 | 2.18 | 0.44 |
| 64:Q:28:LEU:O | 64:Q:65:ILE:N | 2.48 | 0.44 |
| 70:W:75:ILE:HD11 | 70:W:125:ILE:CD1 | 2.48 | 0.44 |
| 83:1:104:ASP:HA | 83:1:105:SER:HB2 | 1.99 | 0.44 |
| 81:2:1315:G:N2 | 81:2:1316:C:C2 | 2.86 | 0.44 |
| 82:4:6159:G:N1 | 82:4:6160:G:C6 | 2.85 | 0.44 |
| 1:5:1493:U:H4' | 1:5:1494:U:OP2 | 2.17 | 0.44 |
| 1:5:1614:U:OP1 | 10:GG:67:ARG:NH2 | 61.92 | 0.44 |
| 1:5:2657:A:N3 | 1:5:2657:A:H2' | 2.32 | 0.44 |
| 1:5:3188:G:N1 | 1:5:3189:C:C4 | 2.86 | 0.44 |
| 1:5:3249:U:H2' | 1:5:3250:U:O4' | 2.18 | 0.44 |
| 1:5:3255:C:H2' | 1:5:3256:A:C5' | 2.48 | 0.44 |
| 1:5:617:G:O6 | 1:5:2836:U:OP1 | 2.35 | 0.44 |
| 5:BB:283:TYR:HB2 | 5:BB:323:ILE:CG2 | 2.45 | 0.44 |
| 6:CC:39:PHE:CD2 | 6:CC:242:ALA:HB2 | 2.53 | 0.44 |
| 3:8:27:U:H4' | 6:CC:51:ALA:HB3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:OO:173[A]:LYS:O | 17:OO:174[A]:ALA:O | 2.36 | 0.44 |
| 59:L:94:VAL:HG21 | 71:X:12:ALA:HB1 | 1.99 | 0.44 |
| 83:1:693:LEU:HD12 | 83:1:700:ARG:CZ | 2.48 | 0.44 |
| 81:2:908:U:H2' | 81:2:909:C:C5 | 2.53 | 0.44 |
| 81:2:987:A:C2 | 81:2:988:U:N3 | 2.86 | 0.44 |
| 81:2:993:G:H2' | 81:2:994:A:O4' | 2.18 | 0.44 |
| 1:5:1304:C:OP1 | 19:QQ:3:ILE:HD11 | 2.18 | 0.44 |
| 1:5:1477:A:C4 | 1:5:1481:G:O6 | 2.71 | 0.44 |
| 1:5:1496:G:O4' | 1:5:1798:G:H2' | 2.18 | 0.44 |
| 1:5:185:C:N3 | 1:5:232:G:C6 | 2.86 | 0.44 |
| 1:5:2333:G:H22 | 1:5:2365:G:H1' | 1.83 | 0.44 |
| 1:5:2559:A:C6 | 1:5:2560:G:C6 | 3.06 | 0.44 |
| 1:5:3215:G:C6 | 1:5:3216:C:C4 | 3.05 | 0.44 |
| 1:5:528:U:O2 | 1:5:529:U:H5 | 2.01 | 0.44 |
| 1:5:635:U:H2' | 1:5:636:C:C6 | 2.53 | 0.44 |
| 3:8:19:C:H2' | 3:8:20:U:C6 | 2.53 | 0.44 |
| 5:BB:14:LEU:CD2 | 5:BB:17:LEU:HD12 | 2.48 | 0.44 |
| 5:BB:41:VAL:HG11 | 5:BB:194:TRP:CG | 2.53 | 0.44 |
| 1:5:2956:C:O2 | 5:BB:266:ARG:NE | 2.51 | 0.44 |
| 15:MM:63:VAL:HG13 | 15:MM:64:VAL:N | 2.33 | 0.44 |
| 17:OO:86[A]:ARG:CG | 17:OO:86[A]:ARG:O | 2.65 | 0.44 |
| 66:S:134:ARG:NH2 | 81:2:1544:G:N7 | 2.66 | 0.44 |
| 22:TT:25:ILE:HD12 | 22:TT:48:ILE:HD11 | 2.00 | 0.44 |
| 22:TT:57:TYR:O | 22:TT:58:GLN:C | 2.56 | 0.44 |
| 28:ZZ:15:ARG:HB2 | 28:ZZ:79:HIS:HD2 | 1.83 | 0.44 |
| 81:2:1027:C:C2 | 81:2:1029:A:O4' | 2.71 | 0.43 |
| 81:2:108:A:O5' | 81:2:108:A:H8 | 2.01 | 0.43 |
| 81:2:1108:G:O2' | 81:2:1137:A:N1 | 2.48 | 0.43 |
| 81:2:1571:A:O4' | 81:2:1572:G:C2 | 2.71 | 0.43 |
| 81:2:363:G:C2 | 81:2:380:C:N3 | 2.86 | 0.43 |
| 81:2:911:U:O2 | 81:2:911:U:C2' | 2.66 | 0.43 |
| 1:5:166:C:N3 | 1:5:256:G:O6 | 2.51 | 0.43 |
| 1:5:2167:A:N9 | 1:5:2238:U:N1 | 2.66 | 0.43 |
| 1:5:216:G:C2 | 1:5:225:C:C2 | 3.06 | 0.43 |
| 1:5:2694:C:C2 | 1:5:2696:G:C2 | 3.06 | 0.43 |
| 1:5:3225:C:H2' | 1:5:3226:U:O4' | 2.17 | 0.43 |
| 2:7:7:G:OP2 | 7:DD:28:THR:HG21 | 2.18 | 0.43 |
| 3:8:103:G:C6 | 3:8:105:A:C6 | 3.06 | 0.43 |
| 3:8:119:C:C2 | 3:8:135:G:C2 | 3.06 | 0.43 |
| 3:8:83:U:O2 | 27:YY:51:ARG:NH2 | 2.51 | 0.43 |
| 6:CC:292:SER:O | 6:CC:293:THR:HG23 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 6:CC:311:HIS:O | 6:CC:311:HIS:ND1 | 2.50 | 0.43 |
| 1:5:1141:A:OP1 | 9:FF:215:ARG:HA | 2.18 | 0.43 |
| 54:G:188:ARG:NH1 | 81:2:283:G:O6 | 2.50 | 0.43 |
| 57:J:12:TYR:CD1 | 57:J:44:ARG:HA | 2.53 | 0.43 |
| 83:1:162:ARG:HA | 83:1:163:ALA:C | 2.38 | 0.43 |
| 83:1:586:ILE:CD1 | 83:1:708:THR:HG1 | 2.08 | 0.43 |
| 83:1:694:HIS:CD2 | 83:1:695:ALA:O | 2.70 | 0.43 |
| 81:2:1175:G:C2 | 81:2:1176:C:C2 | 3.06 | 0.43 |
| 57:J:170:GLY:HA2 | 81:2:511:A:H4' | 1.79 | 0.43 |
| 81:2:568:C:H1' | 81:2:582:C:H5'' | 1.98 | 0.43 |
| 81:2:642:G:N1 | 81:2:692:C:C2 | 2.86 | 0.43 |
| 1:5:1088:G:C2 | 1:5:1089:C:C2 | 3.06 | 0.43 |
| 1:5:2231:A:N3 | 1:5:2231:A:H2' | 2.33 | 0.43 |
| 1:5:2602:U:C4 | 1:5:2603:A:C5 | 3.05 | 0.43 |
| 1:5:2672:A:O2' | 1:5:2673:A:O5' | 2.36 | 0.43 |
| 1:5:2785:A:H4' | 1:5:2786:U:OP2 | 2.18 | 0.43 |
| 1:5:3206:A:H2' | 1:5:3207:G:O4' | 2.18 | 0.43 |
| 1:5:53:G:N2 | 1:5:54:C:C2 | 2.86 | 0.43 |
| 48:A:25:GLY:O | 48:A:26:ALA:HB3 | 2.19 | 0.43 |
| 49:B:222:LYS:O | 49:B:223:PHE:C | 2.56 | 0.43 |
| 50:C:58:ILE:HG23 | 50:C:61:ILE:HD12 | 2.00 | 0.43 |
| 7:DD:148:VAL:HG22 | 7:DD:159:ILE:HG21 | 2.00 | 0.43 |
| 9:FF:80:LEU:HD11 | 9:FF:113:PHE:CD1 | 2.53 | 0.43 |
| 19:QQ:71:LEU:HG | 19:QQ:81:ILE:HD11 | 2.00 | 0.43 |
| 83:1:285:PHE:CE1 | 83:1:320:LEU:HD11 | 2.53 | 0.43 |
| 83:1:587:TYR:CD2 | 83:1:690:ASP:CA | 2.80 | 0.43 |
| 83:1:735:CYS:O | 83:1:766:PHE:N | 2.51 | 0.43 |
| 81:2:1307:G:C6 | 81:2:1308:C:N4 | 2.86 | 0.43 |
| 81:2:1431:G:H2' | 81:2:1432:U:O4' | 2.18 | 0.43 |
| 81:2:1638:C:O2' | 81:2:1760:A:N1 | 2.46 | 0.43 |
| 81:2:561:G:N2 | 81:2:583:C:C2 | 2.87 | 0.43 |
| 81:2:921:G:C6 | 81:2:922:A:C6 | 3.06 | 0.43 |
| 82:4:6211:U:O2' | 82:4:6212:U:H4' | 2.17 | 0.43 |
| 1:5:23:A:H2' | 1:5:24:A:O4' | 2.17 | 0.43 |
| 1:5:3121:U:O2 | 1:5:3121:U:O4' | 2.36 | 0.43 |
| 1:5:3207:G:C2 | 1:5:3208:C:C2 | 3.06 | 0.43 |
| 1:5:488:G:C2 | 1:5:547:A:C2 | 3.06 | 0.43 |
| 1:5:597:G:N1 | 1:5:598:G:C5 | 2.86 | 0.43 |
| 5:BB:57:VAL:CG2 | 5:BB:73:VAL:HG22 | 2.47 | 0.43 |
| 14:LL:75:PHE:O | 14:LL:79:GLU:HB2 | 2.17 | 0.43 |
| 17:OO:149[A]:LYS:HB2 | 17:OO:150[A]:TYR:CE1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 17:OO:77[A]:PRO:HD3 | 17:OO:143[A]:SER:HB3 | 2.00 | 0.43 |
| 72:Y:33:ALA:HB1 | 81:2:531:U:O2' | 2.18 | 0.43 |
| 27:YY:54:ASP:HB2 | 27:YY:70:VAL:N | 2.33 | 0.43 |
| 83:1:481:MET:HA | 83:1:482:LYS:HB2 | 2.01 | 0.43 |
| 83:1:687:ASN:CG | 83:1:688:ILE:HA | 2.39 | 0.43 |
| 81:2:1075:A:C2 | 81:2:1076:C:C6 | 3.05 | 0.43 |
| 81:2:1321:A:H2' | 81:2:1322:C:C6 | 2.53 | 0.43 |
| 81:2:1482:G:C6 | 81:2:1483:C:N4 | 2.86 | 0.43 |
| 81:2:157:U:H4' | 81:2:158:U:OP1 | 2.18 | 0.43 |
| 81:2:403:G:C2 | 81:2:404:C:C2 | 3.07 | 0.43 |
| 1:5:1111:G:C6 | 1:5:1112:C:C4 | 3.07 | 0.43 |
| 1:5:118:U:C5 | 1:5:119:U:C4 | 3.06 | 0.43 |
| 1:5:1604:G:C2 | 1:5:1608:C:C2 | 3.06 | 0.43 |
| 1:5:2438:G:O2' | 1:5:2439:C:O5' | 2.30 | 0.43 |
| 1:5:2540:A:HO2' | 1:5:2541:C:P | 2.26 | 0.43 |
| 1:5:2793:C:C5 | 1:5:2794:U:C5 | 3.07 | 0.43 |
| 1:5:2996:G:H5' | 83:1:27:HIS:CE1 | 2.53 | 0.43 |
| 1:5:482:G:C2 | 1:5:483:C:C2 | 3.07 | 0.43 |
| 1:5:883:G:H2' | 1:5:885:A:N7 | 2.34 | 0.43 |
| 48:A:148:ASP:OD1 | 48:A:151:SER:N | 2.50 | 0.43 |
| 48:A:149:LEU:N | 48:A:149:LEU:HD12 | 2.34 | 0.43 |
| 4:AA:196:TRP:CG | 4:AA:197:PRO:N | 2.87 | 0.43 |
| 49:B:168:ILE:HG12 | 49:B:197:ILE:HG23 | 2.00 | 0.43 |
| 9:FF:153:ILE:HD12 | 9:FF:158:ILE:HB | 1.99 | 0.43 |
| 58:K:15:LEU:HD11 | 58:K:46:LEU:HD21 | 2.00 | 0.43 |
| 17:OO:40[A]:GLU:HG2 | 17:OO:40[A]:GLU:O | 2.16 | 0.43 |
| 6:CC:31:ARG:NH2 | 19:QQ:23:ASN:OD1 | 2.51 | 0.43 |
| 21:SS:106:LEU:HD22 | 21:SS:123:ILE:HD11 | 2.01 | 0.43 |
| 83:1:247:ASP:CB | 83:1:248:SER:HA | 2.48 | 0.43 |
| 81:2:975:G:N1 | 81:2:1022:A:O2' | 2.47 | 0.43 |
| 81:2:14:C:O2 | 81:2:1140:G:C2 | 2.71 | 0.43 |
| 81:2:11:A:N1 | 81:2:1142:A:C2 | 2.87 | 0.43 |
| 81:2:1666:G:C6 | 81:2:1667:U:C4 | 3.07 | 0.43 |
| 81:2:364:G:C6 | 81:2:376:G:C2 | 3.06 | 0.43 |
| 81:2:50:C:N3 | 81:2:429:G:C6 | 2.86 | 0.43 |
| 82:4:6127:C:C4 | 82:4:6160:G:O6 | 2.71 | 0.43 |
| 1:5:1106:A:C6 | 1:5:1107:A:N7 | 2.87 | 0.43 |
| 1:5:1151:A:C2 | 1:5:1153:A:C4 | 3.07 | 0.43 |
| 1:5:1317:G:C5 | 1:5:1318:U:C4 | 3.06 | 0.43 |
| 1:5:1641:U:C2' | 1:5:1642:G:H5' | 2.49 | 0.43 |
| 1:5:2060:U:H4' | 1:5:2061:A:O5' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:5:2218:G:O2' | 1:5:2219:G:C3' | 2.66 | 0.43 |
| 1:5:2237:U:H3' | 1:5:2238:U:H3' | 2.00 | 0.43 |
| 1:5:2694:C:O5' | 1:5:2694:C:O2 | 2.35 | 0.43 |
| 1:5:3114:G:H2' | 1:5:3115:A:C8 | 2.53 | 0.43 |
| 4:AA:133:TYR:CG | 4:AA:168:VAL:HG22 | 2.54 | 0.43 |
| 1:5:887:G:C6 | 4:AA:207:VAL:HG21 | 2.53 | 0.43 |
| 5:BB:75:ALA:O | 5:BB:76:VAL:HG23 | 2.18 | 0.43 |
| 6:CC:138:ARG:NH2 | 6:CC:240:PRO:HG2 | 2.33 | 0.43 |
| 8:EE:51:VAL:HG23 | 8:EE:65:GLY:HA2 | 2.00 | 0.43 |
| 9:FF:205:SER:OG | 9:FF:206:ASN:N | 2.51 | 0.43 |
| 63:P:60:LEU:HD13 | 63:P:89:MET:HG3 | 2.00 | 0.43 |
| 18:PP:69:ARG:HG2 | 18:PP:79:THR:HB | 1.99 | 0.43 |
| 72:Y:29:HIS:O | 72:Y:32:ARG:N | 2.52 | 0.43 |
| 83:1:383:SER:CA | 83:1:465:LYS:O | 2.66 | 0.43 |
| 83:1:686:VAL:O | 83:1:686:VAL:HG13 | 2.19 | 0.43 |
| 83:1:586:ILE:HG22 | 83:1:688:ILE:HD11 | 2.00 | 0.43 |
| 81:2:1670:G:H2' | 81:2:1671:G:H8 | 1.83 | 0.43 |
| 81:2:887:U:O4 | 81:2:888:U:C4 | 2.71 | 0.43 |
| 81:2:8:U:O2' | 81:2:9:U:H5'' | 2.19 | 0.43 |
| 1:5:958:U:C2 | 1:5:1033:A:C2 | 3.07 | 0.43 |
| 1:5:1178:G:C2 | 1:5:1269:C:O2 | 2.71 | 0.43 |
| 1:5:1249:A:C8 | 1:5:1250:C:C5 | 3.07 | 0.43 |
| 1:5:1603:G:N7 | 28:ZZ:17:ARG:NH2 | 2.67 | 0.43 |
| 1:5:1713:G:C2 | 1:5:1714:C:C2 | 3.06 | 0.43 |
| 1:5:2890:G:H5'' | 1:5:2890:G:H8 | 1.84 | 0.43 |
| 1:5:2974:A:H2' | 1:5:2975:U:O4' | 2.19 | 0.43 |
| 1:5:883:G:C2 | 1:5:885:A:C2 | 3.07 | 0.43 |
| 1:5:2506:U:O5' | 49:B:226:GLY:O | 2.36 | 0.43 |
| 5:BB:114:VAL:O | 5:BB:115:LYS:C | 2.55 | 0.43 |
| 5:BB:229:VAL:HG11 | 5:BB:249:VAL:CG2 | 2.43 | 0.43 |
| 5:BB:57:VAL:HB | 5:BB:358:TRP:HB3 | 2.00 | 0.43 |
| 8:EE:127:LYS:O | 8:EE:128:GLU:HG3 | 2.19 | 0.43 |
| 63:P:52:LYS:HB2 | 63:P:53:PRO:HD3 | 1.99 | 0.43 |
| 20:RR:24:MET:CE | 20:RR:32:ILE:HG21 | 2.49 | 0.43 |
| 70:W:8:ALA:HB2 | 70:W:74:VAL:HG11 | 1.99 | 0.43 |
| 28:ZZ:53:VAL:HG12 | 28:ZZ:54:THR:N | 2.33 | 0.43 |
| 83:1:30:HIS:HE1 | 83:1:133:GLU:OE1 | 1.94 | 0.43 |
| 83:1:696:ASP:CB | 83:1:698:ILE:HG23 | 2.47 | 0.43 |
| 81:2:1131:A:C2 | 81:2:1132:A:C5 | 3.06 | 0.43 |
| 81:2:208:U:H2' | 81:2:209:A:O4' | 2.19 | 0.43 |
| 81:2:303:U:H2' | 81:2:304:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 81:2:441:C:N3 | 81:2:442:C:C5 | 2.87 | 0.43 |
| 81:2:734:A:H2' | 81:2:735:C:C6 | 2.54 | 0.43 |
| 81:2:798:A:C2 | 81:2:799:U:C2 | 3.06 | 0.43 |
| 82:4:6172:A:H4' | 82:4:6173:C:OP2 | 2.18 | 0.43 |
| 1:5:1077:G:H2' | 1:5:1078:C:O4' | 2.19 | 0.43 |
| 1:5:1194:A:C6 | 1:5:1195:C:C4 | 3.06 | 0.43 |
| 1:5:1288:A:H2' | 1:5:1288:A:N3 | 2.33 | 0.43 |
| 1:5:1306:C:H2' | 1:5:1307:C:C6 | 2.54 | 0.43 |
| 1:5:1536:A:C2 | 1:5:1544:A:N3 | 2.87 | 0.43 |
| 1:5:1554:C:C3' | 1:5:1555:G:H5' | 2.48 | 0.43 |
| 1:5:1624:G:C5' | 1:5:1624:G:H8 | 2.29 | 0.43 |
| 1:5:1926:U:O4 | 1:5:2054:U:N3 | 2.51 | 0.43 |
| 1:5:2220:G:C6 | 1:5:2221:A:C5 | 3.07 | 0.43 |
| 1:5:2502:G:H3' | 1:5:2503:G:C8 | 2.54 | 0.43 |
| 1:5:3133:A:C2 | 1:5:3254:G:C2 | 3.06 | 0.43 |
| 1:5:3215:G:C4 | 1:5:3216:C:C5 | 3.07 | 0.43 |
| 1:5:634:G:C6 | 1:5:773:C:C2 | 3.07 | 0.43 |
| 1:5:783:G:C2 | 1:5:900:A:C2 | 3.07 | 0.43 |
| 1:5:899:C:H2' | 1:5:900:A:C8 | 2.53 | 0.43 |
| 6:CC:162:THR:HG22 | 6:CC:218:ALA:O | 2.19 | 0.43 |
| 51:D:186:VAL:HG12 | 51:D:188:ILE:CD1 | 2.49 | 0.43 |
| 53:F:63:TYR:CE1 | 53:F:167:LEU:HD11 | 2.54 | 0.43 |
| 10:GG:194:SER:O | 10:GG:196:VAL:N | 2.48 | 0.43 |
| 11:HH:91:ARG:HG3 | 11:HH:182:SER:HB3 | 1.99 | 0.43 |
| 12:II:190:ILE:HG23 | 12:II:197:VAL:CG2 | 2.49 | 0.43 |
| 17:OO:164[A]:ARG:O | 17:OO:168[A]:TYR:N | 2.52 | 0.43 |
| 83:1:78:TYR:HB3 | 83:1:79:SER:CB | 2.49 | 0.43 |
| 81:2:1075:A:C6 | 81:2:1076:C:C5 | 3.07 | 0.43 |
| 81:2:108:A:C6 | 81:2:109:G:C6 | 3.06 | 0.43 |
| 81:2:328:G:C4 | 81:2:329:G:C8 | 3.06 | 0.43 |
| 1:5:1026:A:H4' | 2:7:100:C:O2 | 2.19 | 0.43 |
| 1:5:1637:G:H2' | 1:5:1638:C:O4' | 2.18 | 0.43 |
| 1:5:1929:G:OP1 | 1:5:2032:U:OP1 | 2.37 | 0.43 |
| 1:5:2170:G:C5 | 1:5:2171:C:C4 | 3.06 | 0.43 |
| 1:5:2218:G:O6 | 1:5:2219:G:C2 | 2.71 | 0.43 |
| 1:5:2510:U:C2' | 1:5:2510:U:O2 | 2.67 | 0.43 |
| 1:5:2529:C:C2' | 1:5:2529:C:O2 | 2.67 | 0.43 |
| 1:5:2540:A:O2' | 1:5:2541:C:P | 2.75 | 0.43 |
| 1:5:2654:A:O2' | 7:DD:5:LYS:NZ | 2.52 | 0.43 |
| 1:5:3019:U:C2 | 1:5:3020:G:C8 | 3.07 | 0.43 |
| 1:5:3054:A:C5 | 1:5:3055:A:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:5:1197:G:C5' | 1:5:3085:C:H1' | 2.49 | 0.43 |
| 1:5:3150:G:H2' | 1:5:3151:A:O4' | 2.18 | 0.43 |
| 1:5:3232:G:C2 | 1:5:3233:C:C2 | 3.07 | 0.43 |
| 1:5:637:U:H2' | 1:5:638:A:C8 | 2.54 | 0.43 |
| 1:5:967:A:N3 | 2:7:80:G:O2' | 2.51 | 0.43 |
| 4:AA:201:GLY:O | 4:AA:204:MET:N | 2.52 | 0.43 |
| 4:AA:32:LEU:N | 4:AA:32:LEU:HD23 | 2.33 | 0.43 |
| 6:CC:105:THR:O | 6:CC:109:TRP:NE1 | 2.51 | 0.43 |
| 1:5:1304:C:H1' | 9:FF:206:ASN:OD1 | 2.19 | 0.43 |
| 13:JJ:40:LEU:HD23 | 13:JJ:114:ILE:HD11 | 2.01 | 0.43 |
| 61:N:127:ARG:NH2 | 81:2:628:U:OP1 | 2.51 | 0.43 |
| 17:OO:49[A]:PHE:HE1 | 17:OO:53[A]:LEU:CD1 | 2.32 | 0.43 |
| 19:QQ:34:ALA:HA | 19:QQ:49:LEU:HD13 | 2.01 | 0.43 |
| 20:RR:106:LEU:CD1 | 20:RR:138:LEU:HD21 | 2.49 | 0.43 |
| 24:VV:34:LEU:HD21 | 24:VV:102:ILE:CG2 | 2.47 | 0.43 |
| 83:1:30:HIS:NE2 | 83:1:133:GLU:OE1 | 2.52 | 0.43 |
| 83:1:587:TYR:HB2 | 83:1:689:LEU:H | 1.83 | 0.43 |
| 81:2:1730:A:H2' | 81:2:1731:C:C6 | 2.53 | 0.43 |
| 24:VV:32:ARG:O | 81:2:1733:U:OP1 | 2.36 | 0.43 |
| 81:2:38:C:H2' | 81:2:39:A:O4' | 2.18 | 0.43 |
| 1:5:1193:G:C5 | 1:5:1194:A:N6 | 2.87 | 0.43 |
| 1:5:1496:G:C8 | 1:5:1798:G:C5 | 3.07 | 0.43 |
| 1:5:1679:C:C2 | 1:5:1704:G:N2 | 2.87 | 0.43 |
| 1:5:2154:G:H2' | 1:5:2155:U:O5' | 2.18 | 0.43 |
| 1:5:2237:U:H3' | 1:5:2238:U:C5' | 2.49 | 0.43 |
| 1:5:2240:A:H2' | 1:5:2241:G:O4' | 2.19 | 0.43 |
| 1:5:2908:A:OP2 | 5:BB:2:SER:N | 2.52 | 0.43 |
| 1:5:2959:A:N3 | 18:PP:69:ARG:NH2 | 2.67 | 0.43 |
| 1:5:3043:G:C6 | 1:5:3044:C:C4 | 3.07 | 0.43 |
| 1:5:335:G:C6 | 1:5:336:A:N7 | 2.87 | 0.43 |
| 48:A:32:HIS:HB2 | 81:2:1039:G:O3' | 2.19 | 0.43 |
| 48:A:53:THR:HA | 48:A:161:PRO:HD2 | 1.99 | 0.43 |
| 4:AA:102:LEU:N | 4:AA:102:LEU:HD23 | 2.33 | 0.43 |
| 4:AA:103:PRO:O | 4:AA:105:GLY:N | 2.52 | 0.43 |
| 49:B:38:PHE:CD2 | 49:B:73:LEU:HD13 | 2.54 | 0.43 |
| 6:CC:248:VAL:HG11 | 6:CC:250:TRP:CE2 | 2.53 | 0.43 |
| 3:8:27:U:OP1 | 6:CC:53:SER:CB | 2.66 | 0.43 |
| 17:OO:35[A]:VAL:HG23 | 17:OO:104[A]:LYS:HB2 | 2.01 | 0.43 |
| 83:1:487:PRO:CB | 83:1:488:VAL:HA | 2.49 | 0.43 |
| 83:1:828:MET:CB | 83:1:829:LYS:HA | 2.48 | 0.43 |
| 81:2:1038:A:P | 81:2:1038:A:H3' | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 81:2:1173:C:C2 | 81:2:1464:G:C2 | 3.07 | 0.43 |
| 81:2:1667:U:H2' | 81:2:1668:G:O4' | 2.19 | 0.43 |
| 81:2:1727:C:H2' | 81:2:1728:A:O4' | 2.18 | 0.43 |
| 81:2:48:G:C2 | 81:2:49:C:C2 | 3.07 | 0.43 |
| 81:2:647:G:N3 | 81:2:647:G:H2' | 2.34 | 0.43 |
| 81:2:98:U:H2' | 81:2:99:C:C6 | 2.53 | 0.43 |
| 82:4:6182:A:OP2 | 83:1:585:ARG:CZ | 2.63 | 0.43 |
| 1:5:128:G:C2 | 1:5:141:C:C2 | 3.06 | 0.43 |
| 1:5:1528:A:C5 | 1:5:1530:A:C5 | 3.07 | 0.43 |
| 1:5:1573:U:C2' | 1:5:1573:U:O2 | 2.67 | 0.43 |
| 1:5:1628:U:H2' | 1:5:1629:C:C6 | 2.54 | 0.43 |
| 1:5:2200:C:O2 | 1:5:2200:C:O5' | 2.37 | 0.43 |
| 1:5:29:C:C2 | 1:5:56:G:N2 | 2.87 | 0.43 |
| 1:5:301:G:C6 | 1:5:302:U:C4 | 3.07 | 0.43 |
| 1:5:3048:G:C6 | 1:5:3049:C:C4 | 3.06 | 0.43 |
| 1:5:3192:G:C6 | 1:5:3193:C:C4 | 3.07 | 0.43 |
| 1:5:3228:G:C2 | 1:5:3229:C:C2 | 3.07 | 0.43 |
| 1:5:406:G:H1' | 3:8:16:G:N2 | 2.34 | 0.43 |
| 1:5:664:A:N1 | 3:8:28:C:O2' | 2.39 | 0.43 |
| 1:5:793:G:C6 | 1:5:794:C:C4 | 3.07 | 0.43 |
| 3:8:31:G:C6 | 3:8:32:C:C4 | 3.07 | 0.43 |
| 48:A:54:TRP:HA | 48:A:57:ILE:HD12 | 2.01 | 0.43 |
| 5:BB:218:VAL:HB | 5:BB:337:THR:OG1 | 2.19 | 0.43 |
| 6:CC:121:ALA:HB1 | 6:CC:235:LEU:HD13 | 2.00 | 0.43 |
| 6:CC:319:LYS:O | 6:CC:320:ASN:HB2 | 2.18 | 0.43 |
| 15:MM:15:VAL:HG23 | 15:MM:35:ILE:CD1 | 2.40 | 0.43 |
| 17:OO:95[A]:ARG:O | 17:OO:95[A]:ARG:HG3 | 2.11 | 0.43 |
| 20:RR:136:ARG:O | 20:RR:140:GLU:N | 2.45 | 0.43 |
| 67:T:22:LEU:HD13 | 67:T:28:LEU:HD13 | 2.01 | 0.43 |
| 68:U:95:ALA:HB1 | 68:U:99:ILE:HG21 | 2.01 | 0.43 |
| 69:V:19:ALA:CB | 69:V:59:ILE:HD13 | 2.49 | 0.43 |
| 81:2:1113:G:O2' | 81:2:1129:G:O6 | 2.33 | 0.42 |
| 81:2:1540:G:C2 | 81:2:1566:C:O2 | 2.72 | 0.42 |
| 81:2:440:A:C2 | 81:2:441:C:C6 | 3.06 | 0.42 |
| 81:2:922:A:N1 | 81:2:923:A:N6 | 2.66 | 0.42 |
| 1:5:1083:A:P | 14:LL:5:LYS:HZ2 | 2.42 | 0.42 |
| 1:5:1202:A:C2 | 1:5:1248:C:C5 | 3.07 | 0.42 |
| 1:5:1925:G:C5 | 1:5:2056:C:C4 | 3.06 | 0.42 |
| 1:5:2166:C:N4 | 1:5:2211:A:C4 | 2.87 | 0.42 |
| 1:5:2220:G:C5 | 1:5:2221:A:C8 | 3.07 | 0.42 |
| 1:5:2781:A:C6 | 1:5:2782:G:C5 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:2973:A:H5'' | 5:BB:98:GLY:HA3 | 2.00 | 0.42 |
| 1:5:3048:G:C2 | 1:5:3049:C:C2 | 3.07 | 0.42 |
| 1:5:609:C:C4 | 1:5:619:A:C8 | 3.07 | 0.42 |
| 3:8:24:G:OP2 | 27:YY:13:ARG:NH2 | 2.52 | 0.42 |
| 50:C:61:ILE:HA | 50:C:66:LEU:HD12 | 2.00 | 0.42 |
| 54:G:186:ARG:NE | 81:2:268:G:N7 | 2.67 | 0.42 |
| 17:OO:159[A]:GLU:C | 17:OO:161[A]:ARG:N | 2.72 | 0.42 |
| 17:OO:31[A]:GLY:HA2 | 17:OO:102[A]:ARG:NH2 | 2.34 | 0.42 |
| 24:VV:132:ASN:N | 24:VV:132:ASN:HD22 | 2.17 | 0.42 |
| 27:YY:100:HIS:CG | 27:YY:101:PRO:HD2 | 2.54 | 0.42 |
| 28:ZZ:13:VAL:HG23 | 28:ZZ:23:VAL:HG11 | 2.00 | 0.42 |
| 81:2:1324:A:C2 | 81:2:1325:A:C5 | 3.08 | 0.42 |
| 81:2:274:C:N4 | 81:2:275:C:N4 | 2.68 | 0.42 |
| 81:2:899:A:N1 | 81:2:909:C:C4 | 2.87 | 0.42 |
| 81:2:89:G:C6 | 81:2:90:C:C4 | 3.07 | 0.42 |
| 81:2:922:A:C6 | 81:2:923:A:N6 | 2.87 | 0.42 |
| 81:2:1000:A:OP1 | 82:4:6211:U:H1' | 2.19 | 0.42 |
| 1:5:1157:G:C2 | 1:5:1158:C:C2 | 3.07 | 0.42 |
| 1:5:1282:G:C2 | 1:5:1283:C:C2 | 3.07 | 0.42 |
| 1:5:1290:G:C2 | 1:5:1291:C:C2 | 3.07 | 0.42 |
| 1:5:1397:C:C2 | 1:5:1398:U:C6 | 3.06 | 0.42 |
| 1:5:1565:C:O2' | 1:5:1665:A:N3 | 2.41 | 0.42 |
| 1:5:1927:G:N7 | 1:5:2054:U:O2 | 2.52 | 0.42 |
| 1:5:2530:A:N7 | 10:GG:31:ARG:NH2 | 2.67 | 0.42 |
| 1:5:2634:C:OP2 | 1:5:2655:G:N1 | 2.44 | 0.42 |
| 1:5:2663:A:N1 | 1:5:2727:U:C4 | 2.87 | 0.42 |
| 1:5:3104:G:C6 | 1:5:3105:C:C4 | 3.07 | 0.42 |
| 1:5:3228:G:C6 | 1:5:3229:C:C4 | 3.07 | 0.42 |
| 1:5:340:C:C2 | 3:8:25:G:C2 | 3.07 | 0.42 |
| 1:5:533:G:N1 | 1:5:534:C:C2 | 2.86 | 0.42 |
| 3:8:6:U:C2' | 3:8:7:U:H5' | 2.49 | 0.42 |
| 5:BB:117:ARG:HG2 | 5:BB:178:LEU:HD12 | 2.01 | 0.42 |
| 50:C:186:SER:HB3 | 81:2:4:C:H4' | 2.01 | 0.42 |
| 50:C:56:SER:N | 50:C:60:GLU:OE2 | 2.52 | 0.42 |
| 6:CC:342:LYS:O | 6:CC:344:VAL:N | 2.52 | 0.42 |
| 17:OO:139[A]:LEU:O | 17:OO:141[A]:LYS:CA | 2.64 | 0.42 |
| 1:5:756:G:OP2 | 19:QQ:66:ARG:NH1 | 2.53 | 0.42 |
| 67:T:52:GLY:O | 67:T:54:PHE:N | 2.51 | 0.42 |
| 83:1:247:ASP:HB2 | 83:1:248:SER:HA | 2.01 | 0.42 |
| 81:2:1008:U:H2' | 81:2:1009:C:C6 | 2.55 | 0.42 |
| 81:2:1652:G:N2 | 81:2:1745:G:C6 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-----------------------|--------------------------|-------------------|
| 81:2:19:A:H2' | 81:2:20:G:O4' | 2.19 | 0.42 |
| 81:2:594:G:C2 | 81:2:595:C:N3 | 2.87 | 0.42 |
| 81:2:628:U:N3 | 81:2:629:A:C8 | 2.87 | 0.42 |
| 82:4:6039:A:C2' | 82:4:6039:A:N3 | 2.75 | 0.42 |
| 1:5:1192:A:HO2' | 1:5:1256:G:H1 | 1.62 | 0.42 |
| 1:5:1495:A:C4 | 1:5:1498:C:C4 | 3.08 | 0.42 |
| 1:5:173:G:C5 | 1:5:174:C:C4 | 3.07 | 0.42 |
| 1:5:2228:A:H4' | 1:5:2229:U:OP1 | 2.20 | 0.42 |
| 1:5:2345:G:H2' | 1:5:2346:G:C8 | 2.54 | 0.42 |
| 1:5:2378:G:H4' | 1:5:2379:U:OP2 | 2.19 | 0.42 |
| 1:5:2544:G:C2 | 1:5:2545:C:C2 | 3.07 | 0.42 |
| 1:5:2664:A:H2' | 1:5:2665:A:C8 | 2.53 | 0.42 |
| 1:5:2807:G:N1 | 1:5:2808:C:C4 | 2.87 | 0.42 |
| 1:5:3222:G:C2 | 1:5:3223:U:C2 | 3.08 | 0.42 |
| 1:5:482:G:C6 | 1:5:483:C:C4 | 3.08 | 0.42 |
| 1:5:701:G:C2 | 1:5:702:C:C2 | 3.07 | 0.42 |
| 6:CC:349:ILE:HA | 6:CC:349:ILE:HD12 | 1.94 | 0.42 |
| 61:N:89:TYR:CZ | 61:N:93:LYS:HD2 | 2.54 | 0.42 |
| 17:OO:109[A]:VAL:HA | 17:OO:110[A]:PRO:HD3 | 1.53 | 0.42 |
| 17:OO:11[A]:ASP:O | 17:OO:12[A]:GLY:C | 2.57 | 0.42 |
| 17:OO:146[A]:VAL:O | 17:OO:146[A]:VAL:HG23 | 2.18 | 0.42 |
| 17:OO:182[A]:LYS:O | 17:OO:185[A]:THR:N | 2.52 | 0.42 |
| 70:W:75:ILE:HA | 81:2:1099:G:O2' | 2.19 | 0.42 |
| 59:L:97:TYR:CE1 | 71:X:15:LEU:HB3 | 2.54 | 0.42 |
| 83:1:586:ILE:O | 83:1:587:TYR:CD1 | 2.73 | 0.42 |
| 81:2:1013:G:C5 | 81:2:1014:U:C5 | 3.07 | 0.42 |
| 81:2:1292:U:C4 | 81:2:1293:G:C5 | 3.07 | 0.42 |
| 56:I:58:LEU:HD11 | 81:2:1674:U:OP1 | 2.19 | 0.42 |
| 81:2:1782:C:H2' | 81:2:1783:U:C6 | 2.54 | 0.42 |
| 81:2:623:G:C8 | 81:2:1026:A:C6 | 3.08 | 0.42 |
| 1:5:1092:U:H2' | 1:5:1093:U:O4' | 2.20 | 0.42 |
| 1:5:1350:G:C6 | 1:5:1399:A:C2 | 3.07 | 0.42 |
| 1:5:1425:A:N3 | 1:5:1425:A:C5' | 2.83 | 0.42 |
| 1:5:2326:A:H2' | 1:5:2327:A:C8 | 2.54 | 0.42 |
| 1:5:2459:C:H2' | 1:5:2460:A:O4' | 2.19 | 0.42 |
| 1:5:2504:A:H2' | 1:5:2505:A:O4' | 2.19 | 0.42 |
| 1:5:2592:G:N2 | 1:5:2593:C:C2 | 2.87 | 0.42 |
| 1:5:355:A:H2' | 1:5:356:C:O4' | 2.18 | 0.42 |
| 1:5:488:G:C5 | 1:5:489:G:C6 | 3.07 | 0.42 |
| 1:5:601:A:C2 | 1:5:602:A:C5 | 3.08 | 0.42 |
| 1:5:80:G:N2 | 1:5:81:C:C2 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:8:114:G:C6 | 3:8:115:C:C4 | 3.07 | 0.42 |
| 48:A:195:TRP:CE2 | 48:A:197:ILE:HG21 | 2.53 | 0.42 |
| 52:E:116:ASP:HB2 | 52:E:117:GLU:HB2 | 2.02 | 0.42 |
| 19:QQ:177:GLY:O | 19:QQ:178:ARG:HD3 | 2.20 | 0.42 |
| 83:1:694:HIS:CG | 83:1:695:ALA:O | 2.72 | 0.42 |
| 81:2:1540:G:N1 | 81:2:1566:C:C2 | 2.87 | 0.42 |
| 81:2:1546:G:C2 | 81:2:1547:C:C2 | 3.07 | 0.42 |
| 55:H:112:ARG:NH1 | 81:2:637:U:O2' | 2.53 | 0.42 |
| 82:4:6134:C:H2' | 82:4:6135:C:C6 | 2.54 | 0.42 |
| 1:5:1030:G:C6 | 1:5:1031:U:C4 | 3.08 | 0.42 |
| 1:5:1160:C:C4 | 17:OO:134[A]:ARG:CZ | 3.02 | 0.42 |
| 1:5:1197:G:C2 | 1:5:1198:C:N3 | 2.87 | 0.42 |
| 1:5:1352:A:C2 | 1:5:1397:C:C2 | 3.07 | 0.42 |
| 1:5:1452:A:C2' | 1:5:1827:A:N3 | 2.83 | 0.42 |
| 1:5:1733:G:H3' | 1:5:1734:U:H5'' | 2.02 | 0.42 |
| 1:5:1846:U:H5'' | 1:5:1847:G:O4' | 2.20 | 0.42 |
| 1:5:2077:C:C4 | 1:5:2078:U:C4 | 3.07 | 0.42 |
| 1:5:2149:G:H2' | 1:5:2150:C:C6 | 2.54 | 0.42 |
| 1:5:2236:C:N4 | 1:5:2241:G:C2 | 2.88 | 0.42 |
| 1:5:2238:U:C2' | 1:5:2239:A:O5' | 2.67 | 0.42 |
| 1:5:2816:G:C6 | 1:5:2817:C:C4 | 3.07 | 0.42 |
| 1:5:342:A:N1 | 1:5:349:A:O2' | 2.44 | 0.42 |
| 1:5:586:G:C2 | 1:5:587:C:C2 | 3.07 | 0.42 |
| 3:8:7:U:C4 | 3:8:8:C:C4 | 3.08 | 0.42 |
| 5:BB:324:LEU:HD13 | 5:BB:328:ILE:HD11 | 2.01 | 0.42 |
| 6:CC:138:ARG:O | 6:CC:138:ARG:HD3 | 2.19 | 0.42 |
| 9:FF:52:TYR:CE2 | 9:FF:138:TYR:CE2 | 3.07 | 0.42 |
| 17:OO:23[A]:THR:O | 17:OO:26[A]:LYS:N | 2.53 | 0.42 |
| 17:OO:78[A]:SER:OG | 17:OO:79[A]:ARG:N | 2.52 | 0.42 |
| 19:QQ:157:PRO:HA | 19:QQ:158:HIS:HA | 1.90 | 0.42 |
| 22:TT:12:ARG:HD3 | 22:TT:13:TYR:CZ | 2.55 | 0.42 |
| 28:ZZ:55:LYS:O | 28:ZZ:56:ARG:CB | 2.67 | 0.42 |
| 83:1:560:VAL:CB | 83:1:561:VAL:HA | 2.49 | 0.42 |
| 81:2:1178:G:C2 | 81:2:1179:C:C2 | 3.08 | 0.42 |
| 81:2:506:U:O2 | 81:2:506:U:O4' | 2.37 | 0.42 |
| 81:2:624:C:H2' | 81:2:625:U:C6 | 2.54 | 0.42 |
| 1:5:1354:G:C6 | 1:5:1355:U:C4 | 3.07 | 0.42 |
| 1:5:1495:A:C2 | 1:5:1498:C:C6 | 3.08 | 0.42 |
| 1:5:1572:A:OP1 | 20:RR:38:ARG:NH1 | 2.52 | 0.42 |
| 1:5:1713:G:C6 | 1:5:1714:C:C4 | 3.08 | 0.42 |
| 1:5:2168:G:C5 | 1:5:2169:U:C4 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 1:5:2731:U:C5 | 1:5:2732:C:C5 | 3.07 | 0.42 |
| 1:5:3220:G:O2' | 1:5:3221:G:OP1 | 2.29 | 0.42 |
| 1:5:412:G:H2' | 1:5:413:U:H5' | 2.00 | 0.42 |
| 1:5:494:A:N6 | 1:5:543:A:C2 | 2.87 | 0.42 |
| 1:5:8:C:H2' | 1:5:9:U:O4' | 2.20 | 0.42 |
| 3:8:31:G:C2 | 3:8:32:C:C2 | 3.08 | 0.42 |
| 50:C:232:PRO:HA | 50:C:235:TRP:CD2 | 2.55 | 0.42 |
| 6:CC:346:GLN:O | 6:CC:347:ALA:C | 2.54 | 0.42 |
| 10:GG:147:ALA:HA | 10:GG:200:THR:HG22 | 2.02 | 0.42 |
| 10:GG:162:VAL:O | 10:GG:164:PHE:N | 2.52 | 0.42 |
| 16:NN:189:LYS:O | 16:NN:192:LYS:N | 2.52 | 0.42 |
| 17:OO:16[A]:LEU:HD11 | 17:OO:130[A]:LEU:HD13 | 2.01 | 0.42 |
| 17:OO:23[A]:THR:OG1 | 17:OO:24[A]:VAL:N | 2.53 | 0.42 |
| 18:PP:129:THR:HG21 | 18:PP:139:TYR:CD1 | 2.55 | 0.42 |
| 65:R:31:ASN:HA | 65:R:34:LEU:HD12 | 2.01 | 0.42 |
| 69:V:19:ALA:HB3 | 69:V:59:ILE:HD13 | 2.00 | 0.42 |
| 71:X:42:PRO:O | 71:X:79:ASN:ND2 | 2.53 | 0.42 |
| 28:ZZ:25:ILE:HG23 | 28:ZZ:41:ALA:HB1 | 2.01 | 0.42 |
| 83:1:685:ARG:N | 83:1:686:VAL:HA | 2.34 | 0.42 |
| 83:1:583:HIS:NE2 | 83:1:704:GLN:NE2 | 2.67 | 0.42 |
| 81:2:1437:C:H2' | 81:2:1438:C:C6 | 2.54 | 0.42 |
| 81:2:898:G:H2' | 81:2:899:A:C8 | 2.54 | 0.42 |
| 81:2:929:A:OP2 | 81:2:930:C:H5 | 2.02 | 0.42 |
| 81:2:969:A:C4' | 81:2:969:A:C8 | 3.03 | 0.42 |
| 82:4:6199:A:C6 | 82:4:6200:A:C6 | 3.08 | 0.42 |
| 1:5:1651:U:O4 | 23:UU:90:ARG:NH1 | 2.52 | 0.42 |
| 1:5:1825:C:H2' | 1:5:1826:C:C6 | 2.54 | 0.42 |
| 1:5:2166:C:N3 | 1:5:2211:A:C2 | 2.87 | 0.42 |
| 1:5:412:G:C2' | 1:5:413:U:H5' | 2.50 | 0.42 |
| 1:5:686:U:O2 | 1:5:725:G:H4' | 2.19 | 0.42 |
| 1:5:827:G:C6 | 1:5:828:G:N1 | 2.87 | 0.42 |
| 1:5:930:C:O2 | 1:5:2582:G:O2' | 2.31 | 0.42 |
| 5:BB:25:VAL:HG22 | 5:BB:272:TYR:OH | 2.19 | 0.42 |
| 6:CC:23:PRO:HD2 | 6:CC:26:PHE:CD1 | 2.54 | 0.42 |
| 9:FF:218:LYS:O | 9:FF:219:HIS:HB2 | 2.19 | 0.42 |
| 9:FF:30:ARG:HA | 9:FF:33:ARG:HD2 | 2.02 | 0.42 |
| 54:G:155:ASP:O | 54:G:157:VAL:N | 2.52 | 0.42 |
| 57:J:171:ARG:CA | 81:2:511:A:OP2 | 2.66 | 0.42 |
| 57:J:57:ARG:HG3 | 57:J:97:LEU:HD21 | 2.01 | 0.42 |
| 21:SS:80:ARG:HB3 | 21:SS:124:LEU:HD21 | 2.01 | 0.42 |
| 70:W:125:ILE:HG22 | 70:W:126:LEU:N | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 81:2:1137:A:C4 | 81:2:1138:A:N7 | 2.88 | 0.42 |
| 81:2:1287:G:N7 | 81:2:1313:U:H2' | 2.34 | 0.42 |
| 81:2:1335:A:H2' | 81:2:1336:A:O4' | 2.20 | 0.42 |
| 81:2:1590:A:C2' | 81:2:1591:A:C8 | 2.99 | 0.42 |
| 81:2:906:A:C6 | 81:2:907:U:C5 | 3.08 | 0.42 |
| 81:2:930:C:H3' | 81:2:931:U:H5'' | 2.02 | 0.42 |
| 81:2:957:U:O4' | 81:2:957:U:O2 | 2.37 | 0.42 |
| 82:4:6040:U:H2' | 82:4:6041:C:O5' | 2.19 | 0.42 |
| 1:5:1193:G:H1' | 1:5:1257:A:C2 | 2.54 | 0.42 |
| 1:5:1564:U:H1' | 1:5:1565:C:C6 | 2.55 | 0.42 |
| 1:5:1674:U:O2 | 1:5:1755:G:O2' | 2.38 | 0.42 |
| 1:5:1691:U:O4' | 20:RR:96:ILE:HG12 | 2.19 | 0.42 |
| 1:5:1793:U:H2' | 1:5:1794:G:O4' | 2.19 | 0.42 |
| 1:5:2219:G:C2' | 1:5:2220:G:OP2 | 2.61 | 0.42 |
| 1:5:2236:C:N4 | 1:5:2241:G:N1 | 2.68 | 0.42 |
| 1:5:2823:U:H2' | 1:5:2824:G:O4' | 2.20 | 0.42 |
| 1:5:2852:C:C2 | 1:5:2907:G:N1 | 2.88 | 0.42 |
| 1:5:309:U:C4 | 1:5:310:U:C5 | 3.08 | 0.42 |
| 1:5:837:A:H2' | 1:5:838:G:O4' | 2.20 | 0.42 |
| 3:8:95:A:OP2 | 13:JJ:72:ARG:NH1 | 148.93 | 0.42 |
| 5:BB:294:ALA:HB2 | 5:BB:305:ILE:HG13 | 2.02 | 0.42 |
| 56:I:68:ALA:N | 56:I:186:GLU:OE2 | 2.53 | 0.42 |
| 64:Q:38:LEU:HD11 | 67:T:7:ARG:O | 2.20 | 0.42 |
| 64:Q:9:THR:HA | 81:2:1339:U:O4 | 2.19 | 0.42 |
| 28:ZZ:16:GLY:O | 28:ZZ:18:TYR:N | 2.51 | 0.42 |
| 83:1:119:LEU:HB3 | 83:1:146:ALA:HB2 | 2.02 | 0.42 |
| 83:1:195:GLU:HA | 83:1:196:VAL:HB | 2.00 | 0.42 |
| 83:1:456:LEU:HD13 | 83:1:459:ILE:HD11 | 2.02 | 0.42 |
| 83:1:701:GLY:HA2 | 83:1:703:GLY:N | 2.35 | 0.42 |
| 81:2:1218:A:N6 | 81:2:1263:G:O2' | 2.53 | 0.42 |
| 81:2:1307:G:C6 | 81:2:1308:C:C4 | 3.08 | 0.42 |
| 81:2:391:G:C2 | 81:2:392:C:C2 | 3.08 | 0.42 |
| 81:2:909:C:O2 | 81:2:909:C:C2' | 2.67 | 0.42 |
| 1:5:1925:G:N7 | 1:5:2057:A:C2 | 2.87 | 0.42 |
| 1:5:2055:G:C5 | 1:5:2056:C:N3 | 2.82 | 0.42 |
| 1:5:2169:U:C4 | 1:5:2170:G:N7 | 2.88 | 0.42 |
| 1:5:221:A:C2 | 1:5:224:C:C5 | 3.08 | 0.42 |
| 1:5:2405:U:C2 | 1:5:2480:A:N1 | 2.88 | 0.42 |
| 1:5:271:C:H2' | 1:5:272:G:O4' | 2.19 | 0.42 |
| 1:5:3033:G:H2' | 1:5:3034:U:O4' | 2.20 | 0.42 |
| 1:5:3220:G:O2' | 1:5:3221:G:O4' | 2.38 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:408:A:H2' | 1:5:409:A:O4' | 2.19 | 0.42 |
| 1:5:535:C:H2' | 1:5:536:C:O4' | 2.20 | 0.42 |
| 50:C:183:ILE:HD11 | 50:C:198:VAL:O | 2.19 | 0.42 |
| 6:CC:208:VAL:HA | 6:CC:228:ALA:O | 2.20 | 0.42 |
| 51:D:184:ILE:HD12 | 51:D:184:ILE:N | 2.35 | 0.42 |
| 56:I:9:HIS:O | 56:I:10:LYS:HB2 | 2.20 | 0.42 |
| 57:J:17:ARG:NH2 | 81:2:3:U:O2 | 2.52 | 0.42 |
| 59:L:20:PHE:CG | 81:2:210:U:H5'' | 2.55 | 0.42 |
| 17:OO:107[A]:GLU:C | 17:OO:108[A]:GLY:O | 2.57 | 0.42 |
| 17:OO:40[A]:GLU:HB3 | 17:OO:107[A]:GLU:HB2 | 2.01 | 0.42 |
| 17:OO:77[A]:PRO:HD2 | 17:OO:148[A]:TRP:CG | 2.55 | 0.42 |
| 6:CC:31:ARG:NH2 | 19:QQ:23:ASN:CG | 2.73 | 0.42 |
| 24:VV:33:ASN:C | 24:VV:33:ASN:HD22 | 2.24 | 0.42 |
| 28:ZZ:53:VAL:CG1 | 28:ZZ:54:THR:N | 2.83 | 0.42 |
| 83:1:580:PRO:CA | 83:1:583:HIS:CD2 | 3.03 | 0.42 |
| 83:1:586:ILE:HD11 | 83:1:708:THR:CG2 | 2.50 | 0.42 |
| 83:1:582:LYS:HE3 | 83:1:694:HIS:CE1 | 2.55 | 0.42 |
| 81:2:1014:U:C5 | 81:2:1015:C:N3 | 2.87 | 0.42 |
| 81:2:1292:U:C4 | 81:2:1293:G:C4 | 3.08 | 0.42 |
| 81:2:884:G:H2' | 81:2:885:U:C6 | 2.55 | 0.42 |
| 1:5:1192:A:O2' | 1:5:1193:G:OP2 | 2.38 | 0.42 |
| 1:5:1192:A:O2' | 1:5:1256:G:N1 | 2.45 | 0.42 |
| 1:5:2055:G:C2 | 1:5:2056:C:C2 | 3.08 | 0.42 |
| 1:5:2061:A:C6 | 1:5:2062:A:N6 | 2.88 | 0.42 |
| 1:5:2150:C:H2' | 1:5:2151:A:O4' | 2.20 | 0.42 |
| 1:5:217:U:C2' | 1:5:218:G:OP1 | 2.68 | 0.42 |
| 1:5:470:G:C6 | 1:5:471:C:C4 | 3.07 | 0.42 |
| 1:5:917:U:H2' | 1:5:918:G:H8 | 1.85 | 0.42 |
| 48:A:23:HIS:CG | 48:A:50:VAL:HG22 | 2.54 | 0.42 |
| 1:5:2506:U:OP1 | 49:B:230:SER:HB3 | 2.20 | 0.42 |
| 50:C:46:LEU:CD2 | 50:C:73:ILE:HD13 | 2.49 | 0.42 |
| 7:DD:116:ASP:OD1 | 7:DD:116:ASP:N | 2.53 | 0.42 |
| 57:J:170:GLY:N | 81:2:510:A:O3' | 2.46 | 0.42 |
| 15:MM:21:VAL:HG12 | 15:MM:65:LEU:HA | 2.01 | 0.42 |
| 64:Q:120:ASP:O | 64:Q:123:ARG:NH1 | 2.53 | 0.42 |
| 7:DD:34:LYS:HA | 22:TT:27:LEU:HD11 | 2.02 | 0.42 |
| 24:VV:46:LEU:HD13 | 24:VV:47:ASN:HB2 | 2.01 | 0.42 |
| 1:5:2541:C:H5'' | 28:ZZ:58:GLY:HA3 | 2.02 | 0.42 |
| 28:ZZ:40:HIS:HD2 | 28:ZZ:74:VAL:HG13 | 1.82 | 0.42 |
| 83:1:338:ILE:HA | 83:1:342:LEU:HD12 | 2.02 | 0.41 |
| 83:1:33:SER:CA | 83:1:57:THR:HG21 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|---------------------|--------------------------|-------------------|
| 83:1:405:VAL:HA | 83:1:406:LYS:CG | 2.50 | 0.41 |
| 83:1:587:TYR:C | 83:1:588:LEU:HG | 2.39 | 0.41 |
| 81:2:1093:G:H2' | 81:2:1094:U:O5' | 2.20 | 0.41 |
| 81:2:1417:G:C2 | 81:2:1418:C:O2 | 2.73 | 0.41 |
| 81:2:161:A:C6 | 81:2:162:G:C6 | 3.08 | 0.41 |
| 81:2:255:A:H2' | 81:2:256:A:O4' | 2.20 | 0.41 |
| 81:2:429:G:C6 | 81:2:430:C:C4 | 3.08 | 0.41 |
| 81:2:429:G:C2 | 81:2:430:C:C2 | 3.08 | 0.41 |
| 81:2:886:A:C2' | 81:2:887:U:O4' | 2.68 | 0.41 |
| 81:2:958:U:O2 | 81:2:958:U:H2' | 2.20 | 0.41 |
| 82:4:6181:C:O2 | 82:4:6196:A:C2 | 2.73 | 0.41 |
| 1:5:1312:U:H2' | 1:5:1313:C:C6 | 2.55 | 0.41 |
| 1:5:1372:G:N1 | 1:5:1373:C:C4 | 2.88 | 0.41 |
| 1:5:1522:C:H2' | 1:5:1523:G:O4' | 2.20 | 0.41 |
| 1:5:1633:G:C6 | 1:5:1634:C:C4 | 3.08 | 0.41 |
| 1:5:1688:G:H2' | 1:5:1689:U:O4' | 2.19 | 0.41 |
| 1:5:1722:G:N1 | 1:5:1723:C:C2 | 2.88 | 0.41 |
| 1:5:18:G:C6 | 1:5:19:U:C4 | 3.08 | 0.41 |
| 1:5:1910:C:H2' | 1:5:1911:U:C6 | 2.55 | 0.41 |
| 1:5:2236:C:C5 | 1:5:2237:U:C5 | 3.08 | 0.41 |
| 1:5:29:C:C2 | 1:5:56:G:C2 | 3.08 | 0.41 |
| 1:5:642:U:H2' | 1:5:643:C:O4' | 2.20 | 0.41 |
| 2:7:95:A:C6 | 2:7:96:U:C4 | 3.08 | 0.41 |
| 3:8:76:C:H2' | 3:8:77:A:O4' | 2.20 | 0.41 |
| 48:A:23:HIS:NE2 | 48:A:50:VAL:HG13 | 2.35 | 0.41 |
| 4:AA:237:LEU:HD12 | 4:AA:243:THR:CG2 | 2.49 | 0.41 |
| 7:DD:140:ARG:HB3 | 7:DD:141:PRO:HD2 | 2.02 | 0.41 |
| 8:EE:127:LYS:HZ1 | 18:PP:173:ARG:HH12 | 1.67 | 0.41 |
| 55:H:162:ILE:HD13 | 55:H:169:PHE:CE2 | 2.55 | 0.41 |
| 13:JJ:110:ILE:HG22 | 13:JJ:116:TYR:HA | 2.01 | 0.41 |
| 59:L:91:LEU:HD13 | 59:L:100:TYR:CB | 2.49 | 0.41 |
| 17:OO:127[A]:VAL:HG12 | 17:OO:128[A]:LEU:HG | 2.02 | 0.41 |
| 27:YY:49:PRO:O | 27:YY:115:ARG:NH2 | 2.53 | 0.41 |
| 83:1:380:LEU:HB2 | 83:1:399:ARG:O | 2.20 | 0.41 |
| 83:1:380:LEU:HB3 | 83:1:401:PHE:H | 1.84 | 0.41 |
| 83:1:42:ARG:HA | 83:1:43:ALA:C | 2.41 | 0.41 |
| 83:1:441:PHE:HB2 | 83:1:442:VAL:CB | 2.50 | 0.41 |
| 83:1:647:ILE:CG1 | 83:1:685:ARG:NH1 | 2.84 | 0.41 |
| 81:2:1460:G:C2 | 81:2:1461:C:C2 | 3.08 | 0.41 |
| 81:2:1493:C:C2 | 81:2:1511:G:N2 | 2.88 | 0.41 |
| 81:2:208:U:C4 | 81:2:209:A:N7 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 81:2:941:G:C6 | 81:2:942:C:C4 | 3.08 | 0.41 |
| 1:5:109:A:H4' | 1:5:110:G:OP1 | 2.19 | 0.41 |
| 1:5:1197:G:C6 | 1:5:1198:C:C4 | 3.08 | 0.41 |
| 1:5:1397:C:H2' | 1:5:1397:C:O2 | 2.19 | 0.41 |
| 1:5:2671:A:N6 | 7:DD:150:LEU:HD11 | 2.34 | 0.41 |
| 1:5:2781:A:N6 | 1:5:2782:G:C6 | 2.88 | 0.41 |
| 1:5:2886:G:C2 | 1:5:2897:C:C2 | 3.08 | 0.41 |
| 1:5:2939:A:H2' | 1:5:2939:A:N3 | 2.35 | 0.41 |
| 1:5:3224:G:C6 | 1:5:3225:C:C2 | 3.08 | 0.41 |
| 1:5:533:G:C5 | 1:5:534:C:C5 | 3.07 | 0.41 |
| 1:5:623:C:H2' | 1:5:624:G:C8 | 2.55 | 0.41 |
| 1:5:851:G:OP2 | 18:PP:131:ARG:HA | 2.20 | 0.41 |
| 2:7:87:G:OP1 | 9:FF:215:ARG:NH1 | 2.52 | 0.41 |
| 3:8:116:G:N2 | 3:8:117:C:C2 | 2.88 | 0.41 |
| 48:A:90:ALA:HB2 | 48:A:97:PRO:CG | 2.49 | 0.41 |
| 6:CC:349:ILE:HG23 | 6:CC:350:LYS:CE | 2.42 | 0.41 |
| 3:8:27:U:OP1 | 6:CC:53:SER:HB2 | 2.20 | 0.41 |
| 11:HH:4:ILE:HD12 | 21:SS:143:PHE:HE1 | 1.85 | 0.41 |
| 11:HH:89:LYS:HG2 | 11:HH:145:VAL:HG22 | 2.02 | 0.41 |
| 12:II:65:LEU:HD11 | 12:II:91:VAL:HG13 | 2.01 | 0.41 |
| 1:5:1464:G:O6 | 14:LL:2:ALA:N | 66.60 | 0.41 |
| 17:OO:171[A]:LYS:CB | 17:OO:171[A]:LYS:HZ2 | 2.33 | 0.41 |
| 83:1:36:THR:HB | 83:1:102:LEU:HD11 | 2.01 | 0.41 |
| 81:2:9:U:H2' | 81:2:11:A:OP2 | 2.20 | 0.41 |
| 63:P:47:ARG:NE | 81:2:1551:G:N7 | 2.67 | 0.41 |
| 81:2:1637:C:H2' | 81:2:1638:C:O4' | 2.20 | 0.41 |
| 81:2:284:G:C2 | 81:2:285:C:C2 | 3.08 | 0.41 |
| 81:2:284:G:C6 | 81:2:285:C:C4 | 3.08 | 0.41 |
| 81:2:579:A:C6 | 81:2:582:C:C6 | 3.08 | 0.41 |
| 81:2:859:U:H2' | 81:2:860:U:O4' | 2.20 | 0.41 |
| 81:2:886:A:C6 | 81:2:887:U:C4 | 3.08 | 0.41 |
| 81:2:969:A:C8 | 81:2:969:A:C3' | 3.03 | 0.41 |
| 81:2:924:G:N2 | 81:2:987:A:C8 | 2.89 | 0.41 |
| 82:4:6181:C:C3' | 83:1:578:LYS:HZ1 | 2.28 | 0.41 |
| 82:4:6172:A:OP2 | 82:4:6200:A:N6 | 2.53 | 0.41 |
| 1:5:109:A:C6 | 1:5:323:A:C4 | 3.08 | 0.41 |
| 1:5:1742:C:H2' | 1:5:1743:C:O4' | 2.20 | 0.41 |
| 1:5:1918:A:OP2 | 20:RR:135:LYS:NZ | 2.54 | 0.41 |
| 1:5:2991:U:C5 | 1:5:2999:G:N2 | 2.88 | 0.41 |
| 1:5:3139:U:H3' | 1:5:3140:A:H5'' | 2.00 | 0.41 |
| 1:5:982:A:O4' | 12:II:194:GLY:HA3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:A:202:TYR:O | 48:A:205:ARG:NH1 | 2.54 | 0.41 |
| 9:FF:86:ILE:CD1 | 9:FF:211:TRP:CZ3 | 3.03 | 0.41 |
| 18:PP:158:GLU:HA | 18:PP:159:LYS:CB | 2.50 | 0.41 |
| 23:UU:89:LEU:HB3 | 23:UU:93:ILE:HD12 | 2.02 | 0.41 |
| 83:1:701:GLY:CA | 83:1:702:GLY:C | 2.88 | 0.41 |
| 83:1:733:ILE:HD12 | 83:1:743:ILE:CD1 | 2.51 | 0.41 |
| 83:1:735:CYS:HB3 | 83:1:740:VAL:HG11 | 2.01 | 0.41 |
| 81:2:1482:G:C2 | 81:2:1483:C:N3 | 2.88 | 0.41 |
| 81:2:571:C:C4 | 81:2:572:C:C5 | 3.08 | 0.41 |
| 81:2:566:A:C2 | 81:2:582:C:H1' | 2.55 | 0.41 |
| 81:2:828:A:O2' | 81:2:829:U:OP2 | 2.38 | 0.41 |
| 81:2:945:U:H2' | 81:2:946:U:N1 | 2.36 | 0.41 |
| 81:2:952:G:H2' | 81:2:953:G:C8 | 2.56 | 0.41 |
| 1:5:1074:A:N3 | 1:5:1074:A:H2' | 2.35 | 0.41 |
| 1:5:1091:A:C2 | 1:5:1110:G:C2 | 3.08 | 0.41 |
| 1:5:1108:C:C4 | 1:5:1109:U:C5 | 3.09 | 0.41 |
| 1:5:1928:A:C6 | 1:5:2053:C:C2 | 3.09 | 0.41 |
| 1:5:2093:G:C2 | 1:5:2299:C:C2 | 3.09 | 0.41 |
| 1:5:248:U:O2 | 1:5:248:U:C2' | 2.64 | 0.41 |
| 1:5:2852:C:C2 | 1:5:2907:G:C2 | 3.08 | 0.41 |
| 1:5:3037:G:O2' | 20:RR:61:SER:CB | 2.68 | 0.41 |
| 1:5:323:A:N6 | 1:5:324:A:N1 | 2.68 | 0.41 |
| 1:5:385:A:C2 | 1:5:386:A:C4 | 3.07 | 0.41 |
| 1:5:532:A:N7 | 1:5:533:G:C8 | 2.88 | 0.41 |
| 2:7:87:G:OP1 | 9:FF:215:ARG:HD3 | 2.20 | 0.41 |
| 54:G:136:LYS:NZ | 54:G:174:LYS:O | 2.54 | 0.41 |
| 57:J:45:ILE:HG12 | 57:J:104:PHE:HB3 | 2.02 | 0.41 |
| 16:NN:150:TRP:CZ3 | 16:NN:151:ILE:HG12 | 2.55 | 0.41 |
| 24:VV:13:ILE:CD1 | 24:VV:54:LEU:HB3 | 2.50 | 0.41 |
| 83:1:517:CYS:SG | 83:1:537:HIS:NE2 | 2.94 | 0.41 |
| 83:1:638:PRO:HA | 83:1:639:ASP:HA | 1.87 | 0.41 |
| 81:2:1130:A:H2' | 81:2:1131:A:O4' | 2.20 | 0.41 |
| 81:2:992:A:N6 | 81:2:993:G:N3 | 2.69 | 0.41 |
| 1:5:1297:A:H2' | 1:5:1298:C:O4' | 2.21 | 0.41 |
| 1:5:1503:C:O2 | 1:5:1560:G:C2 | 2.73 | 0.41 |
| 1:5:1678:C:N3 | 1:5:1705:G:C2 | 2.89 | 0.41 |
| 1:5:1749:G:C6 | 1:5:1750:C:N4 | 2.88 | 0.41 |
| 1:5:2218:G:O2' | 1:5:2219:G:C4' | 2.69 | 0.41 |
| 1:5:2530:A:C1' | 1:5:2531:A:OP1 | 2.67 | 0.41 |
| 1:5:909:C:O2' | 1:5:2782:G:O2' | 2.36 | 0.41 |
| 1:5:287:G:C6 | 1:5:288:C:N3 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 1:5:3192:G:C2 | 1:5:3193:C:C2 | 3.08 | 0.41 |
| 1:5:825:G:O2' | 20:RR:130:ASN:ND2 | 2.54 | 0.41 |
| 1:5:835:G:O6 | 1:5:864:C:H3' | 2.21 | 0.41 |
| 3:8:116:G:C2 | 3:8:117:C:C2 | 3.08 | 0.41 |
| 5:BB:56:ILE:CD1 | 5:BB:76:VAL:HG21 | 2.45 | 0.41 |
| 6:CC:230:VAL:HG22 | 6:CC:254:ALA:HB1 | 2.02 | 0.41 |
| 52:E:86:PHE:O | 52:E:87:MET:HB2 | 2.20 | 0.41 |
| 56:I:83:TYR:CZ | 56:I:196:ARG:HG2 | 2.55 | 0.41 |
| 57:J:131:GLN:O | 57:J:133:HIS:CD2 | 2.74 | 0.41 |
| 17:OO:126[A]:ARG:CG | 17:OO:126[A]:ARG:O | 2.66 | 0.41 |
| 17:OO:186[A]:VAL:C | 17:OO:187[A]:GLY:O | 2.58 | 0.41 |
| 17:OO:46[A]:GLY:HA3 | 17:OO:51[A]:ASN:HD21 | 1.86 | 0.41 |
| 17:OO:76[A]:ALA:HA | 17:OO:77[A]:PRO:HD2 | 1.90 | 0.41 |
| 17:OO:77[A]:PRO:HG2 | 17:OO:148[A]:TRP:CZ2 | 2.56 | 0.41 |
| 18:PP:22:LEU:HD12 | 18:PP:146:ILE:CD1 | 2.50 | 0.41 |
| 21:SS:29:ILE:HG22 | 21:SS:31:ALA:HB2 | 2.03 | 0.41 |
| 83:1:219:ALA:HB3 | 83:1:330:ALA:HA | 2.02 | 0.41 |
| 83:1:441:PHE:HB2 | 83:1:442:VAL:CA | 2.50 | 0.41 |
| 83:1:464:LEU:HD12 | 83:1:464:LEU:HA | 1.89 | 0.41 |
| 81:2:1127:C:H2' | 81:2:1128:U:O4' | 2.20 | 0.41 |
| 81:2:1177:G:H3' | 81:2:1178:G:H8 | 1.86 | 0.41 |
| 81:2:1666:G:H2' | 81:2:1667:U:O4' | 2.20 | 0.41 |
| 81:2:22:A:HO2' | 81:2:23:G:C5' | 2.30 | 0.41 |
| 81:2:284:G:N1 | 81:2:285:C:C4 | 2.88 | 0.41 |
| 81:2:334:U:H2' | 81:2:335:G:O4' | 2.21 | 0.41 |
| 81:2:585:G:C6 | 81:2:586:C:C4 | 3.08 | 0.41 |
| 1:5:1017:A:H2' | 1:5:1020:C:C5 | 2.55 | 0.41 |
| 1:5:1119:G:C2 | 1:5:1127:C:N3 | 2.89 | 0.41 |
| 1:5:1196:A:H3' | 1:5:1197:G:C8 | 2.56 | 0.41 |
| 1:5:1587:G:O2' | 3:8:126:A:N1 | 2.54 | 0.41 |
| 1:5:1604:G:N2 | 1:5:1608:C:C2 | 2.88 | 0.41 |
| 1:5:1909:G:C6 | 1:5:1910:C:N3 | 2.88 | 0.41 |
| 1:5:2729:G:C4 | 1:5:2763:U:C5 | 3.08 | 0.41 |
| 1:5:3302:U:H4' | 1:5:3303:A:C5' | 2.51 | 0.41 |
| 3:8:107:G:C6 | 3:8:108:C:C4 | 3.08 | 0.41 |
| 49:B:157:GLN:O | 49:B:158:SER:C | 2.59 | 0.41 |
| 5:BB:77:THR:HG23 | 5:BB:326:GLY:O | 2.19 | 0.41 |
| 17:OO:145[A]:SER:O | 17:OO:145[A]:SER:OG | 2.37 | 0.41 |
| 83:1:586:ILE:O | 83:1:587:TYR:CG | 2.73 | 0.41 |
| 81:2:1707:C:O2 | 81:2:1707:C:O4' | 2.38 | 0.41 |
| 81:2:1750:U:O4 | 81:2:1751:A:N6 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|---------------------|--------------------------|-------------------|
| 81:2:362:G:C2 | 81:2:381:C:C2 | 3.09 | 0.41 |
| 81:2:509:G:C6 | 81:2:510:A:N7 | 2.88 | 0.41 |
| 81:2:826:C:H2' | 81:2:827:U:C6 | 2.55 | 0.41 |
| 81:2:989:C:O2 | 81:2:989:C:O5' | 2.38 | 0.41 |
| 19:QQ:124:LEU:HG | 82:4:6039:A:H1' | 119.65 | 0.41 |
| 1:5:1195:C:C5 | 1:5:1196:A:C8 | 3.09 | 0.41 |
| 1:5:1290:G:C6 | 1:5:1291:C:C4 | 3.08 | 0.41 |
| 1:5:157:A:H2' | 1:5:158:G:O4' | 2.20 | 0.41 |
| 1:5:2050:A:H2' | 1:5:2050:A:N3 | 2.36 | 0.41 |
| 1:5:2218:G:C1' | 1:5:2219:G:C5' | 2.84 | 0.41 |
| 1:5:2802:G:C2 | 1:5:2823:U:C2 | 3.09 | 0.41 |
| 1:5:3215:G:C6 | 1:5:3216:C:N4 | 2.88 | 0.41 |
| 1:5:3274:U:C2' | 1:5:3275:A:H5'' | 2.51 | 0.41 |
| 6:CC:230:VAL:CG2 | 6:CC:254:ALA:HB1 | 2.50 | 0.41 |
| 9:FF:236:LEU:HD21 | 9:FF:240:MET:SD | 2.61 | 0.41 |
| 56:I:76:THR:CG2 | 56:I:104:ILE:HG23 | 2.50 | 0.41 |
| 8:EE:49:ARG:NH1 | 15:MM:114:ASP:OD2 | 2.53 | 0.41 |
| 17:OO:179[A]:VAL:HG12 | 17:OO:179[A]:VAL:O | 2.21 | 0.41 |
| 17:OO:79[A]:ARG:HA | 17:OO:82[A]:TYR:HB3 | 2.02 | 0.41 |
| 83:1:385:MET:HG3 | 83:1:394:PHE:CE2 | 2.55 | 0.41 |
| 83:1:53:GLU:HA | 83:1:54:ALA:HB3 | 2.01 | 0.41 |
| 81:2:1211:G:O2' | 81:2:1240:G:N2 | 2.54 | 0.41 |
| 81:2:1726:U:H2' | 81:2:1727:C:C6 | 2.56 | 0.41 |
| 81:2:1752:A:H5'' | 81:2:1752:A:H8 | 1.85 | 0.41 |
| 81:2:979:G:C6 | 81:2:980:U:C4 | 3.08 | 0.41 |
| 82:4:6075:A:H2' | 82:4:6076:U:C6 | 2.56 | 0.41 |
| 82:4:6210:U:H1' | 82:4:6211:U:C5 | 2.56 | 0.41 |
| 1:5:1145:G:C2 | 1:5:1146:C:C2 | 3.08 | 0.41 |
| 1:5:1599:U:H3' | 1:5:1599:U:O2 | 2.21 | 0.41 |
| 1:5:1643:G:C2 | 1:5:1743:C:O2 | 2.74 | 0.41 |
| 1:5:1451:G:O2' | 1:5:1840:U:O4 | 2.27 | 0.41 |
| 1:5:2438:G:C2 | 1:5:2439:C:C2 | 3.09 | 0.41 |
| 1:5:2807:G:C6 | 1:5:2808:C:C4 | 3.09 | 0.41 |
| 1:5:3008:A:H5' | 24:VV:12:ARG:HB2 | 2.02 | 0.41 |
| 1:5:3220:G:C2' | 1:5:3221:G:O4' | 2.67 | 0.41 |
| 1:5:408:A:N6 | 3:8:15:G:H1' | 2.36 | 0.41 |
| 1:5:647:G:C6 | 1:5:648:C:C4 | 3.09 | 0.41 |
| 2:7:112:G:C6 | 2:7:113:C:N4 | 2.88 | 0.41 |
| 48:A:129:ASP:O | 48:A:131:GLN:N | 2.54 | 0.41 |
| 9:FF:138:TYR:O | 9:FF:139:SER:CB | 2.69 | 0.41 |
| 12:II:95:HIS:HB3 | 12:II:126:ALA:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------------|-----------------------|--------------------------|-------------------|
| 14:LL:89:TYR:O | 14:LL:92:THR:OG1 | 2.29 | 0.41 |
| 17:OO:185[A]:THR:HG23 | 17:OO:186[A]:VAL:HG23 | 2.03 | 0.41 |
| 17:OO:70[A]:GLY:O | 17:OO:71[A]:PRO:O | 2.38 | 0.41 |
| 24:VV:81:GLN:O | 24:VV:82:SER:CB | 2.68 | 0.41 |
| 71:X:50:LYS:HG3 | 71:X:103:LEU:HD23 | 2.03 | 0.41 |
| 83:1:107:GLY:CA | 83:1:138:GLN:HE22 | 2.33 | 0.41 |
| 83:1:240:MET:O | 83:1:242:ASP:N | 2.54 | 0.41 |
| 83:1:694:HIS:CG | 83:1:696:ASP:OD1 | 2.70 | 0.41 |
| 81:2:1031:G:C6 | 81:2:1032:C:C4 | 3.09 | 0.41 |
| 81:2:1175:G:C6 | 81:2:1176:C:C4 | 3.09 | 0.41 |
| 81:2:1467:A:H2' | 81:2:1468:C:C6 | 2.56 | 0.41 |
| 81:2:602:U:H2' | 81:2:603:A:O4' | 2.20 | 0.41 |
| 82:4:6133:G:C2' | 82:4:6134:C:C5 | 3.04 | 0.41 |
| 1:5:1124:A:C6 | 1:5:1125:A:N1 | 2.88 | 0.41 |
| 1:5:1451:G:O4' | 1:5:1454:G:N2 | 2.54 | 0.41 |
| 1:5:1811:A:H4' | 1:5:1812:C:OP2 | 2.20 | 0.41 |
| 1:5:1871:G:O5' | 1:5:1871:G:C8 | 2.74 | 0.41 |
| 1:5:2247:C:N4 | 1:5:2276:G:C6 | 2.89 | 0.41 |
| 1:5:2260:A:H2' | 1:5:2261:U:O4' | 2.20 | 0.41 |
| 1:5:2619:G:C2 | 1:5:2764:G:C4 | 3.09 | 0.41 |
| 1:5:2699:U:H2' | 1:5:2700:G:O4' | 2.21 | 0.41 |
| 1:5:3207:G:C6 | 1:5:3208:C:C4 | 3.09 | 0.41 |
| 1:5:533:G:N2 | 1:5:534:C:H1' | 2.35 | 0.41 |
| 1:5:947:U:OP1 | 19:QQ:144:ARG:NH2 | 2.53 | 0.41 |
| 3:8:10:A:C6 | 3:8:11:C:C4 | 3.09 | 0.41 |
| 3:8:140:G:C6 | 3:8:141:C:C4 | 3.08 | 0.41 |
| 5:BB:339:ARG:HG3 | 5:BB:340:LYS:O | 2.21 | 0.41 |
| 6:CC:16:THR:HA | 6:CC:17:SER:HB3 | 2.02 | 0.41 |
| 6:CC:31:ARG:HH11 | 6:CC:31:ARG:HB3 | 1.85 | 0.41 |
| 6:CC:349:ILE:CG2 | 6:CC:350:LYS:HE3 | 2.45 | 0.41 |
| 1:5:1427:A:C4 | 7:DD:64:ILE:HD11 | 155.59 | 0.41 |
| 53:F:134:VAL:HG11 | 53:F:201:ILE:HD12 | 2.03 | 0.41 |
| 59:L:48:ALA:HA | 59:L:53:TYR:OH | 2.20 | 0.41 |
| 17:OO:111[A]:PRO:CB | 17:OO:112[A]:PRO:HD3 | 2.37 | 0.41 |
| 17:OO:13[A]:LYS:HD2 | 17:OO:38[A]:ARG:CZ | 2.45 | 0.41 |
| 70:W:73:GLY:HA3 | 70:W:128:PHE:CE2 | 2.56 | 0.41 |
| 28:ZZ:51:LEU:HB3 | 28:ZZ:65:ARG:HD2 | 2.03 | 0.41 |
| 83:1:149:GLU:N | 83:1:150:ARG:HA | 2.35 | 0.41 |
| 83:1:698:ILE:HD13 | 83:1:700:ARG:HD3 | 1.46 | 0.41 |
| 81:2:523:U:C6 | 81:2:525:A:OP2 | 2.74 | 0.41 |
| 81:2:823:G:C6 | 81:2:848:C:N4 | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 81:2:989:C:H3' | 81:2:990:G:C8 | 2.56 | 0.41 |
| 82:4:6128:A:C2 | 82:4:6159:G:N3 | 2.89 | 0.41 |
| 1:5:1370:A:C2 | 3:8:8:C:C5' | 3.03 | 0.41 |
| 1:5:2086:A:H2' | 1:5:2087:C:O4' | 2.20 | 0.41 |
| 1:5:2218:G:C3' | 1:5:2218:G:OP2 | 2.69 | 0.41 |
| 1:5:2238:U:C2' | 1:5:2239:A:H5' | 2.49 | 0.41 |
| 1:5:2928:C:H2' | 1:5:2929:G:C8 | 2.55 | 0.41 |
| 1:5:312:C:C2 | 1:5:2746:G:N1 | 2.89 | 0.41 |
| 1:5:53:G:C2 | 1:5:54:C:C2 | 3.09 | 0.41 |
| 1:5:584:A:C2 | 1:5:585:U:C2 | 3.09 | 0.41 |
| 1:5:586:G:C6 | 1:5:587:C:C4 | 3.08 | 0.41 |
| 2:7:68:C:H2' | 2:7:69:C:O4' | 2.21 | 0.41 |
| 4:AA:200:ARG:O | 4:AA:203:ALA:N | 2.53 | 0.41 |
| 5:BB:218:VAL:HG13 | 5:BB:274:HIS:CE1 | 2.48 | 0.41 |
| 5:BB:316:ALA:O | 5:BB:317:ILE:HB | 2.21 | 0.41 |
| 50:C:46:LEU:HD12 | 50:C:66:LEU:HD13 | 2.03 | 0.41 |
| 6:CC:206:LEU:HD23 | 6:CC:208:VAL:HG23 | 2.03 | 0.41 |
| 6:CC:92:ASN:O | 6:CC:93:MET:C | 2.59 | 0.41 |
| 8:EE:171:HIS:CD2 | 8:EE:172:LEU:HG | 2.56 | 0.41 |
| 10:GG:135:LEU:HD21 | 10:GG:165:LEU:HD11 | 2.03 | 0.41 |
| 17:OO:26[A]:LYS:HD3 | 17:OO:26[A]:LYS:O | 2.21 | 0.41 |
| 17:OO:93[A]:THR:OG1 | 17:OO:93[A]:THR:O | 2.32 | 0.41 |
| 83:1:693:LEU:HA | 83:1:693:LEU:HD13 | 1.76 | 0.41 |
| 81:2:1482:G:N1 | 81:2:1483:C:C4 | 2.89 | 0.41 |
| 81:2:1773:U:H2' | 81:2:1774:A:C8 | 2.56 | 0.41 |
| 81:2:362:G:H2' | 81:2:363:G:O4' | 2.21 | 0.41 |
| 81:2:630:G:C6 | 81:2:631:U:C4 | 3.09 | 0.41 |
| 1:5:1410:U:H2' | 1:5:1411:G:O4' | 2.20 | 0.41 |
| 1:5:1791:C:O2' | 1:5:1792:A:P | 2.79 | 0.41 |
| 1:5:2236:C:C4 | 1:5:2237:U:C4 | 3.09 | 0.41 |
| 1:5:2339:G:H2' | 1:5:2340:G:O4' | 2.21 | 0.41 |
| 1:5:2482:U:C4 | 1:5:2560:G:C5 | 3.09 | 0.41 |
| 1:5:2799:G:C6 | 1:5:2800:C:C4 | 3.08 | 0.41 |
| 1:5:3006:U:H2' | 1:5:3007:C:O4' | 2.21 | 0.41 |
| 1:5:331:G:H2' | 1:5:332:C:C6 | 2.56 | 0.41 |
| 1:5:336:A:C2 | 3:8:27:U:N3 | 2.83 | 0.41 |
| 1:5:506:G:C2 | 1:5:528:U:O2 | 2.74 | 0.41 |
| 48:A:119:ARG:O | 48:A:120:LEU:HB2 | 2.21 | 0.41 |
| 5:BB:227:GLU:HG2 | 5:BB:270:ARG:HD2 | 2.03 | 0.41 |
| 6:CC:208:VAL:O | 6:CC:251:THR:HG23 | 2.21 | 0.41 |
| 6:CC:26:PHE:HE1 | 6:CC:258:LEU:HD13 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 8:EE:87:THR:HG21 | 15:MM:115:PHE:HB3 | 2.03 | 0.41 |
| 54:G:3:LEU:HD22 | 54:G:111:LEU:HD11 | 2.02 | 0.41 |
| 14:LL:47:ALA:CB | 14:LL:48:PRO:CD | 2.98 | 0.41 |
| 16:NN:38:ARG:CZ | 16:NN:60:VAL:HG13 | 2.51 | 0.41 |
| 17:OO:82[A]:TYR:CZ | 17:OO:100[A]:LEU:HD13 | 2.56 | 0.41 |
| 17:OO:136[A]:TYR:HD1 | 17:OO:136[A]:TYR:H | 1.69 | 0.41 |
| 17:OO:139[A]:LEU:C | 17:OO:141[A]:LYS:H | 2.21 | 0.41 |
| 18:PP:165:VAL:O | 18:PP:167:ARG:N | 2.54 | 0.41 |
| 24:VV:35:TYR:CG | 24:VV:63:LYS:HE2 | 2.55 | 0.41 |
| 81:2:1154:G:N2 | 81:2:1622:C:C2 | 2.89 | 0.40 |
| 81:2:1320:A:H4' | 81:2:1321:A:OP1 | 2.20 | 0.40 |
| 81:2:1464:G:C6 | 81:2:1465:C:C4 | 3.10 | 0.40 |
| 81:2:1473:A:H2' | 81:2:1474:C:O4' | 2.21 | 0.40 |
| 56:I:5:ARG:NE | 81:2:335:G:O6 | 2.43 | 0.40 |
| 81:2:524:A:C6 | 81:2:525:A:C6 | 3.08 | 0.40 |
| 81:2:94:U:H2' | 81:2:95:G:O4' | 2.21 | 0.40 |
| 82:4:6133:G:O2' | 82:4:6134:C:C6 | 2.70 | 0.40 |
| 1:5:922:A:H5'' | 1:5:1114:A:N1 | 2.36 | 0.40 |
| 1:5:1546:G:C6 | 1:5:1547:C:N4 | 2.89 | 0.40 |
| 1:5:2218:G:O2' | 1:5:2219:G:C5' | 2.69 | 0.40 |
| 1:5:2276:G:H3' | 1:5:2277:C:H5'' | 2.03 | 0.40 |
| 1:5:258:G:C2 | 1:5:259:C:C2 | 3.08 | 0.40 |
| 1:5:2662:A:N1 | 1:5:2663:A:C2 | 2.89 | 0.40 |
| 1:5:2807:G:C2 | 1:5:2808:C:C2 | 3.09 | 0.40 |
| 1:5:307:A:C2 | 1:5:308:A:C5 | 3.09 | 0.40 |
| 1:5:3055:A:O4' | 1:5:3343:A:N1 | 2.54 | 0.40 |
| 1:5:377:A:H1' | 1:5:392:G:N2 | 2.35 | 0.40 |
| 1:5:507:U:O4' | 1:5:532:A:N3 | 2.53 | 0.40 |
| 1:5:521:U:H2' | 1:5:522:A:N9 | 2.36 | 0.40 |
| 1:5:563:G:O6 | 1:5:584:A:H3' | 2.21 | 0.40 |
| 1:5:670:G:H2' | 1:5:671:U:C6 | 2.56 | 0.40 |
| 2:7:38:U:N3 | 2:7:41:G:OP2 | 2.52 | 0.40 |
| 50:C:188:ALA:HB2 | 50:C:212:LEU:HD11 | 2.03 | 0.40 |
| 6:CC:206:LEU:HB2 | 6:CC:246:ARG:NE | 2.35 | 0.40 |
| 7:DD:50:ARG:HB2 | 7:DD:147:ASP:OD1 | 2.21 | 0.40 |
| 9:FF:86:ILE:HA | 9:FF:86:ILE:HD13 | 1.94 | 0.40 |
| 17:OO:121[A]:VAL:O | 17:OO:122[A]:PRO:C | 2.60 | 0.40 |
| 17:OO:9[A]:VAL:HG12 | 17:OO:118[A]:ARG:CB | 2.44 | 0.40 |
| 19:QQ:34:ALA:HA | 19:QQ:49:LEU:CD1 | 2.52 | 0.40 |
| 20:RR:143:ILE:O | 20:RR:147:ALA:N | 2.50 | 0.40 |
| 67:T:108:LEU:HB3 | 67:T:114:VAL:HG23 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 71:X:23:ARG:HD2 | 71:X:29:TYR:CD1 | 2.56 | 0.40 |
| 27:YY:54:ASP:HB2 | 27:YY:70:VAL:HB | 2.03 | 0.40 |
| 53:F:122:ILE:HG23 | 73:Z:59:TYR:CE2 | 2.56 | 0.40 |
| 83:1:464:LEU:HG | 83:1:465:LYS:HG3 | 2.03 | 0.40 |
| 83:1:706:ILE:HG23 | 83:1:707:PRO:HD2 | 2.03 | 0.40 |
| 50:C:102:ARG:NH2 | 81:2:1300:U:OP2 | 2.54 | 0.40 |
| 81:2:364:G:C5 | 81:2:376:G:N2 | 2.90 | 0.40 |
| 81:2:384:A:H5'' | 81:2:384:A:C8 | 2.56 | 0.40 |
| 81:2:960:U:H2' | 81:2:961:C:C6 | 2.57 | 0.40 |
| 82:4:6060:U:C5 | 82:4:6062:G:OP1 | 2.74 | 0.40 |
| 1:5:1019:A:H2' | 12:II:22:TYR:CE2 | 2.57 | 0.40 |
| 1:5:1088:G:C6 | 1:5:1089:C:C4 | 3.10 | 0.40 |
| 1:5:1165:G:C6 | 1:5:1166:A:N6 | 2.88 | 0.40 |
| 1:5:12:A:C2 | 1:5:13:A:N1 | 2.89 | 0.40 |
| 1:5:1333:G:H2' | 1:5:1334:A:H8 | 1.81 | 0.40 |
| 1:5:1886:C:H2' | 1:5:1887:C:O4' | 2.21 | 0.40 |
| 1:5:2163:G:C6 | 1:5:2164:C:C4 | 3.10 | 0.40 |
| 1:5:2235:U:H2' | 1:5:2236:C:H5 | 1.79 | 0.40 |
| 1:5:2479:U:C3' | 1:5:2480:A:H5' | 2.32 | 0.40 |
| 1:5:2544:G:C6 | 1:5:2545:C:C4 | 3.08 | 0.40 |
| 1:5:2592:G:C2 | 1:5:2593:C:N3 | 2.89 | 0.40 |
| 1:5:3200:G:C2 | 1:5:3224:G:C4 | 3.09 | 0.40 |
| 1:5:830:G:C6 | 1:5:832:C:C4 | 3.08 | 0.40 |
| 1:5:930:C:C5 | 1:5:2769:A:C4 | 3.09 | 0.40 |
| 49:B:211:HIS:O | 49:B:212:ILE:HD12 | 2.22 | 0.40 |
| 5:BB:246:LEU:O | 5:BB:248:LYS:N | 2.54 | 0.40 |
| 5:BB:311:PHE:HE2 | 5:BB:317:ILE:HD12 | 1.86 | 0.40 |
| 7:DD:94:ASN:OD1 | 7:DD:94:ASN:N | 2.55 | 0.40 |
| 1:5:3154:A:N6 | 11:HH:58:HIS:O | 2.50 | 0.40 |
| 12:II:174:THR:HA | 12:II:196:PHE:CZ | 2.56 | 0.40 |
| 17:OO:53[A]:LEU:HD23 | 17:OO:53[A]:LEU:HA | 1.80 | 0.40 |
| 20:RR:119:LEU:O | 20:RR:123:LEU:HG | 2.20 | 0.40 |
| 21:SS:7:TYR:CE2 | 21:SS:63:VAL:HG22 | 2.56 | 0.40 |
| 59:L:102:LYS:O | 71:X:13:ARG:NH2 | 2.54 | 0.40 |
| 71:X:7:ARG:NH2 | 81:2:1099:G:C1' | 2.83 | 0.40 |
| 83:1:721:ASP:N | 83:1:722:PRO:HD2 | 2.37 | 0.40 |
| 81:2:1460:G:C6 | 81:2:1461:C:C4 | 3.08 | 0.40 |
| 81:2:1513:A:O2' | 81:2:1516:C:N4 | 2.54 | 0.40 |
| 81:2:326:U:H2' | 81:2:327:A:C8 | 2.56 | 0.40 |
| 81:2:325:G:C2 | 81:2:342:C:C2 | 3.09 | 0.40 |
| 81:2:425:G:C2 | 81:2:426:C:C2 | 3.09 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 81:2:452:U:O2 | 81:2:452:U:H2' | 2.21 | 0.40 |
| 81:2:567:G:C6 | 81:2:568:C:N4 | 2.90 | 0.40 |
| 81:2:854:A:N1 | 81:2:856:U:O2 | 2.55 | 0.40 |
| 82:4:6084:A:N7 | 82:4:6085:G:C8 | 2.89 | 0.40 |
| 1:5:1531:G:C6 | 1:5:1532:G:C6 | 3.09 | 0.40 |
| 1:5:2163:G:C2 | 1:5:2164:C:C4 | 3.09 | 0.40 |
| 1:5:2218:G:C1' | 1:5:2219:G:O4' | 2.70 | 0.40 |
| 1:5:60:A:C4 | 1:5:327:A:C2 | 3.09 | 0.40 |
| 1:5:824:G:H2' | 1:5:825:G:O4' | 2.21 | 0.40 |
| 1:5:847:A:C2 | 1:5:857:C:C2 | 3.10 | 0.40 |
| 48:A:23:HIS:CE1 | 48:A:50:VAL:HG13 | 2.57 | 0.40 |
| 5:BB:6:TYR:O | 5:BB:8:ALA:N | 2.54 | 0.40 |
| 9:FF:80:LEU:HD21 | 9:FF:113:PHE:HB3 | 2.03 | 0.40 |
| 9:FF:128:GLU:N | 9:FF:129:PRO:CD | 2.84 | 0.40 |
| 54:G:153:VAL:HB | 81:2:78:A:C8 | 2.57 | 0.40 |
| 17:OO:114[A]:ASP:CA | 17:OO:118[A]:ARG:HH12 | 2.08 | 0.40 |
| 17:OO:128[A]:LEU:HA | 17:OO:128[A]:LEU:HD23 | 1.79 | 0.40 |
| 1:5:1284:G:O3' | 17:OO:18[A]:GLY:HA3 | 2.21 | 0.40 |
| 17:OO:28[A]:LEU:HD23 | 17:OO:28[A]:LEU:N | 2.23 | 0.40 |
| 20:RR:38:ARG:O | 20:RR:42:ARG:N | 2.48 | 0.40 |
| 26:XX:113:LEU:C | 26:XX:113:LEU:CD1 | 2.88 | 0.40 |
| 28:ZZ:24:VAL:HG11 | 28:ZZ:87:LEU:HD23 | 2.04 | 0.40 |
| 83:1:47:SER:HB2 | 83:1:48:ALA:HB3 | 2.03 | 0.40 |
| 83:1:584:ASN:HB3 | 83:1:692:THR:O | 2.11 | 0.40 |
| 81:2:107:C:H5'' | 81:2:382:G:C2' | 2.52 | 0.40 |
| 82:4:6128:A:C4 | 82:4:6159:G:N2 | 2.89 | 0.40 |
| 1:5:1138:U:H2' | 1:5:1139:U:O4' | 2.21 | 0.40 |
| 1:5:1202:A:O2' | 1:5:1249:A:N6 | 2.53 | 0.40 |
| 1:5:1400:G:OP2 | 6:CC:107:ARG:NH1 | 2.44 | 0.40 |
| 1:5:2249:A:O2' | 1:5:2250:A:H5'' | 2.21 | 0.40 |
| 1:5:286:U:H2' | 1:5:287:G:O4' | 2.22 | 0.40 |
| 1:5:3138:A:C2 | 1:5:3249:U:C2 | 3.09 | 0.40 |
| 1:5:3188:G:C6 | 1:5:3189:C:C4 | 3.10 | 0.40 |
| 1:5:3200:G:H2' | 1:5:3201:C:C6 | 2.56 | 0.40 |
| 1:5:945:G:N2 | 1:5:946:C:C2 | 2.90 | 0.40 |
| 1:5:95:A:C5 | 1:5:96:G:H1' | 2.57 | 0.40 |
| 2:7:79:A:H2' | 2:7:80:G:O4' | 2.22 | 0.40 |
| 1:5:2915:G:C6 | 5:BB:251:CYS:SG | 3.14 | 0.40 |
| 5:BB:252:ILE:HG21 | 5:BB:260:VAL:HG13 | 2.03 | 0.40 |
| 6:CC:349:ILE:CB | 6:CC:350:LYS:HG3 | 2.51 | 0.40 |
| 54:G:155:ASP:H | 81:2:78:A:P | 2.30 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:G:141:ILE:HD11 | 54:G:156:TYR:O | 2.22 | 0.40 |
| 55:H:173:TYR:CZ | 55:H:177:THR:HG21 | 2.55 | 0.40 |
| 16:NN:46:ASP:O | 16:NN:47:LYS:C | 2.59 | 0.40 |
| 64:Q:7:VAL:HG11 | 64:Q:91:ALA:HB1 | 2.03 | 0.40 |
| 22:TT:65:TYR:CE1 | 22:TT:73:GLY:HA3 | 2.56 | 0.40 |
| 70:W:76:SER:OG | 81:2:1100:G:H5' | 2.21 | 0.40 |
| 81:2:1209:C:C2 | 81:2:1452:G:N2 | 2.89 | 0.40 |
| 81:2:207:U:N3 | 81:2:208:U:C4 | 2.90 | 0.40 |
| 81:2:429:G:N2 | 81:2:430:C:C2 | 2.90 | 0.40 |
| 81:2:50:C:OP1 | 81:2:422:G:N2 | 2.53 | 0.40 |
| 81:2:760:A:C6 | 81:2:761:G:C4 | 3.09 | 0.40 |
| 81:2:89:G:C2 | 81:2:90:C:C2 | 3.09 | 0.40 |
| 81:2:929:A:O2' | 81:2:930:C:P | 2.78 | 0.40 |
| 81:2:947:G:C2 | 81:2:948:C:C2 | 3.10 | 0.40 |
| 82:4:6040:U:C5 | 82:4:6041:C:C5 | 3.10 | 0.40 |
| 82:4:6120:U:C2' | 82:4:6120:U:O2 | 2.69 | 0.40 |
| 82:4:6173:C:H2' | 82:4:6173:C:O2 | 2.20 | 0.40 |
| 82:4:6199:A:HO2' | 82:4:6200:A:H5' | 1.69 | 0.40 |
| 1:5:1145:G:N1 | 1:5:1146:C:C4 | 2.90 | 0.40 |
| 1:5:1475:A:C5 | 1:5:1476:C:C5 | 3.10 | 0.40 |
| 1:5:1484:G:O2' | 1:5:1485:G:H5' | 2.21 | 0.40 |
| 1:5:1727:G:C2 | 1:5:1728:C:C2 | 3.10 | 0.40 |
| 1:5:1927:G:C5 | 1:5:2054:U:O2 | 2.75 | 0.40 |
| 1:5:2057:A:O2' | 1:5:2058:A:H5' | 2.21 | 0.40 |
| 1:5:2063:C:H2' | 1:5:2064:G:O4' | 2.21 | 0.40 |
| 1:5:2173:C:N3 | 1:5:2208:G:C6 | 2.90 | 0.40 |
| 1:5:2592:G:C2 | 1:5:2593:C:C2 | 3.10 | 0.40 |
| 1:5:2944:A:N6 | 1:5:2945:G:C6 | 2.89 | 0.40 |
| 1:5:2960:U:H1' | 18:PP:69:ARG:NH2 | 2.37 | 0.40 |
| 1:5:3008:A:C5' | 24:VV:12:ARG:HB2 | 2.51 | 0.40 |
| 1:5:317:A:H2' | 1:5:318:A:C8 | 2.56 | 0.40 |
| 1:5:768:U:H2' | 1:5:769:G:O4' | 2.22 | 0.40 |
| 1:5:781:A:H2' | 1:5:782:U:C6 | 2.57 | 0.40 |
| 49:B:120:LEU:HD12 | 49:B:121:ILE:N | 2.37 | 0.40 |
| 51:D:98:ALA:HA | 51:D:188:ILE:HD13 | 2.04 | 0.40 |
| 58:K:54:PHE:N | 58:K:54:PHE:CD1 | 2.89 | 0.40 |
| 1:5:1870:A:O2' | 24:VV:49:LEU:HD21 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 4 | AA | 247/249 (99%) | 198 (80%) | 35 (14%) | 14 (6%) | 2 | 23 |
| 5 | BB | 382/384 (100%) | 311 (81%) | 52 (14%) | 19 (5%) | 2 | 26 |
| 6 | CC | 357/360 (99%) | 273 (76%) | 57 (16%) | 27 (8%) | 1 | 15 |
| 7 | DD | 293/295 (99%) | 254 (87%) | 27 (9%) | 12 (4%) | 3 | 32 |
| 8 | EE | 157/170 (92%) | 127 (81%) | 22 (14%) | 8 (5%) | 2 | 26 |
| 9 | FF | 220/222 (99%) | 182 (83%) | 25 (11%) | 13 (6%) | 2 | 23 |
| 10 | GG | 231/233 (99%) | 198 (86%) | 25 (11%) | 8 (4%) | 4 | 37 |
| 11 | HH | 189/191 (99%) | 168 (89%) | 19 (10%) | 2 (1%) | 17 | 61 |
| 12 | II | 203/216 (94%) | 179 (88%) | 20 (10%) | 4 (2%) | 9 | 49 |
| 13 | JJ | 166/168 (99%) | 136 (82%) | 20 (12%) | 10 (6%) | 2 | 22 |
| 14 | LL | 195/197 (99%) | 170 (87%) | 17 (9%) | 8 (4%) | 3 | 32 |
| 15 | MM | 134/136 (98%) | 124 (92%) | 5 (4%) | 5 (4%) | 4 | 35 |
| 16 | NN | 200/202 (99%) | 172 (86%) | 25 (12%) | 3 (2%) | 12 | 55 |
| 17 | OO | 196/198 (99%) | 88 (45%) | 40 (20%) | 68 (35%) | 0 | 0 |
| 18 | PP | 178/180 (99%) | 152 (85%) | 19 (11%) | 7 (4%) | 3 | 33 |
| 19 | QQ | 182/184 (99%) | 155 (85%) | 23 (13%) | 4 (2%) | 8 | 47 |
| 20 | RR | 186/188 (99%) | 155 (83%) | 25 (13%) | 6 (3%) | 5 | 38 |
| 21 | SS | 167/169 (99%) | 144 (86%) | 18 (11%) | 5 (3%) | 5 | 40 |
| 22 | TT | 156/158 (99%) | 126 (81%) | 22 (14%) | 8 (5%) | 2 | 26 |
| 23 | UU | 98/100 (98%) | 86 (88%) | 12 (12%) | 0 | 100 | 100 |
| 24 | VV | 130/132 (98%) | 115 (88%) | 10 (8%) | 5 (4%) | 4 | 34 |
| 25 | WW | 60/62 (97%) | 53 (88%) | 7 (12%) | 0 | 100 | 100 |
| 26 | XX | 119/121 (98%) | 107 (90%) | 11 (9%) | 1 (1%) | 22 | 65 |
| 27 | YY | 123/125 (98%) | 104 (85%) | 16 (13%) | 3 (2%) | 7 | 45 |
| 28 | ZZ | 132/134 (98%) | 107 (81%) | 17 (13%) | 8 (6%) | 2 | 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29 | aa | 145/147 (99%) | 121 (83%) | 17 (12%) | 7 (5%) | 2 | 27 |
| 30 | bb | 55/57 (96%) | 48 (87%) | 5 (9%) | 2 (4%) | 4 | 36 |
| 31 | cc | 95/97 (98%) | 83 (87%) | 12 (13%) | 0 | 100 | 100 |
| 32 | dd | 104/106 (98%) | 90 (86%) | 9 (9%) | 5 (5%) | 2 | 27 |
| 33 | ee | 120/122 (98%) | 104 (87%) | 15 (12%) | 1 (1%) | 22 | 65 |
| 34 | ff | 103/105 (98%) | 94 (91%) | 8 (8%) | 1 (1%) | 18 | 62 |
| 35 | gg | 119/121 (98%) | 102 (86%) | 9 (8%) | 8 (7%) | 1 | 20 |
| 36 | hh | 114/116 (98%) | 100 (88%) | 11 (10%) | 3 (3%) | 6 | 43 |
| 37 | ii | 96/98 (98%) | 75 (78%) | 16 (17%) | 5 (5%) | 2 | 25 |
| 38 | jj | 83/85 (98%) | 66 (80%) | 16 (19%) | 1 (1%) | 15 | 59 |
| 39 | kk | 74/76 (97%) | 55 (74%) | 16 (22%) | 3 (4%) | 3 | 32 |
| 40 | ll | 47/49 (96%) | 38 (81%) | 7 (15%) | 2 (4%) | 3 | 30 |
| 41 | mm | 49/51 (96%) | 41 (84%) | 7 (14%) | 1 (2%) | 9 | 49 |
| 42 | nn | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 43 | oo | 99/101 (98%) | 74 (75%) | 21 (21%) | 4 (4%) | 3 | 32 |
| 44 | pp | 85/87 (98%) | 62 (73%) | 14 (16%) | 9 (11%) | 0 | 9 |
| 45 | qq | 215/217 (99%) | 166 (77%) | 33 (15%) | 16 (7%) | 1 | 16 |
| 46 | rr | 193/195 (99%) | 147 (76%) | 30 (16%) | 16 (8%) | 1 | 13 |
| 48 | A | 204/206 (99%) | 160 (78%) | 31 (15%) | 13 (6%) | 1 | 21 |
| 49 | B | 212/214 (99%) | 162 (76%) | 43 (20%) | 7 (3%) | 4 | 38 |
| 50 | C | 215/217 (99%) | 170 (79%) | 34 (16%) | 11 (5%) | 2 | 26 |
| 51 | D | 221/223 (99%) | 190 (86%) | 24 (11%) | 7 (3%) | 5 | 38 |
| 52 | E | 258/260 (99%) | 220 (85%) | 26 (10%) | 12 (5%) | 3 | 28 |
| 53 | F | 204/206 (99%) | 168 (82%) | 29 (14%) | 7 (3%) | 4 | 38 |
| 54 | G | 224/226 (99%) | 188 (84%) | 28 (12%) | 8 (4%) | 4 | 36 |
| 55 | H | 182/184 (99%) | 149 (82%) | 21 (12%) | 12 (7%) | 1 | 20 |
| 56 | I | 184/200 (92%) | 148 (80%) | 29 (16%) | 7 (4%) | 4 | 34 |
| 57 | J | 180/182 (99%) | 151 (84%) | 19 (11%) | 10 (6%) | 2 | 24 |
| 58 | K | 94/96 (98%) | 78 (83%) | 12 (13%) | 4 (4%) | 3 | 30 |
| 59 | L | 153/155 (99%) | 122 (80%) | 24 (16%) | 7 (5%) | 3 | 29 |
| 60 | M | 120/122 (98%) | 94 (78%) | 22 (18%) | 4 (3%) | 4 | 38 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 61 | N | 148/150 (99%) | 129 (87%) | 17 (12%) | 2 (1%) | 13 | 56 |
| 62 | O | 125/127 (98%) | 104 (83%) | 18 (14%) | 3 (2%) | 7 | 45 |
| 63 | P | 121/123 (98%) | 98 (81%) | 16 (13%) | 7 (6%) | 2 | 23 |
| 64 | Q | 139/141 (99%) | 120 (86%) | 12 (9%) | 7 (5%) | 2 | 26 |
| 65 | R | 127/129 (98%) | 99 (78%) | 23 (18%) | 5 (4%) | 3 | 33 |
| 66 | S | 143/145 (99%) | 117 (82%) | 21 (15%) | 5 (4%) | 4 | 37 |
| 67 | T | 141/143 (99%) | 126 (89%) | 13 (9%) | 2 (1%) | 13 | 56 |
| 68 | U | 104/106 (98%) | 92 (88%) | 9 (9%) | 3 (3%) | 5 | 41 |
| 69 | V | 85/87 (98%) | 66 (78%) | 14 (16%) | 5 (6%) | 2 | 23 |
| 70 | W | 127/129 (98%) | 104 (82%) | 18 (14%) | 5 (4%) | 3 | 33 |
| 71 | X | 143/145 (99%) | 112 (78%) | 20 (14%) | 11 (8%) | 1 | 15 |
| 72 | Y | 132/134 (98%) | 111 (84%) | 13 (10%) | 8 (6%) | 2 | 22 |
| 73 | Z | 68/70 (97%) | 57 (84%) | 8 (12%) | 3 (4%) | 3 | 30 |
| 74 | a | 98/100 (98%) | 68 (69%) | 13 (13%) | 17 (17%) | 0 | 3 |
| 75 | b | 80/82 (98%) | 61 (76%) | 15 (19%) | 4 (5%) | 2 | 26 |
| 76 | c | 61/63 (97%) | 56 (92%) | 5 (8%) | 0 | 100 | 100 |
| 77 | d | 51/53 (96%) | 40 (78%) | 11 (22%) | 0 | 100 | 100 |
| 78 | e | 53/55 (96%) | 46 (87%) | 4 (8%) | 3 (6%) | 2 | 23 |
| 79 | f | 67/69 (97%) | 49 (73%) | 12 (18%) | 6 (9%) | 1 | 12 |
| 80 | g | 312/324 (96%) | 251 (80%) | 50 (16%) | 11 (4%) | 4 | 37 |
| 83 | 1 | 825/827 (100%) | 654 (79%) | 120 (14%) | 51 (6%) | 2 | 22 |
| All | All | 12121/12322 (98%) | 9932 (82%) | 1590 (13%) | 599 (5%) | 5 | 27 |

All (599) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AA | 10 | LYS |
| 4 | AA | 34 | TYR |
| 4 | AA | 92 | LYS |
| 4 | AA | 181 | LYS |
| 4 | AA | 197 | PRO |
| 4 | AA | 222 | ALA |
| 5 | BB | 4 | ARG |
| 5 | BB | 222 | LYS |
| 5 | BB | 226 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 5 | BB | 255 | TRP |
| 6 | CC | 23 | PRO |
| 6 | CC | 84 | ARG |
| 6 | CC | 105 | THR |
| 6 | CC | 148 | ILE |
| 6 | CC | 149 | PRO |
| 6 | CC | 182 | VAL |
| 6 | CC | 292 | SER |
| 6 | CC | 352 | SER |
| 6 | CC | 353 | ALA |
| 7 | DD | 20 | PHE |
| 8 | EE | 13 | VAL |
| 8 | EE | 14 | PRO |
| 8 | EE | 66 | PRO |
| 8 | EE | 127 | LYS |
| 8 | EE | 129 | ILE |
| 9 | FF | 90 | ASN |
| 9 | FF | 139 | SER |
| 9 | FF | 156 | GLN |
| 9 | FF | 161 | SER |
| 9 | FF | 214 | PRO |
| 9 | FF | 216 | LYS |
| 9 | FF | 219 | HIS |
| 9 | FF | 230 | GLU |
| 10 | GG | 75 | ALA |
| 10 | GG | 126 | PRO |
| 10 | GG | 163 | ILE |
| 11 | HH | 3 | TYR |
| 12 | II | 24 | ARG |
| 12 | II | 145 | LYS |
| 13 | JJ | 8 | PRO |
| 13 | JJ | 64 | LYS |
| 14 | LL | 3 | ILE |
| 14 | LL | 47 | ALA |
| 16 | NN | 75 | VAL |
| 17 | OO | 20[A] | LEU |
| 17 | OO | 24[A] | VAL |
| 17 | OO | 32[A] | GLN |
| 17 | OO | 34[A] | ILE |
| 17 | OO | 35[A] | VAL |
| 17 | OO | 40[A] | GLU |
| 17 | OO | 42[A] | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 17 | OO | 45[A] | SER |
| 17 | OO | 50[A] | ARG |
| 17 | OO | 51[A] | ASN |
| 17 | OO | 56[A] | HIS |
| 17 | OO | 64[A] | ALA |
| 17 | OO | 66[A] | ASN |
| 17 | OO | 67[A] | LYS |
| 17 | OO | 84[A] | ALA |
| 17 | OO | 86[A] | ARG |
| 17 | OO | 94[A] | ALA |
| 17 | OO | 95[A] | ARG |
| 17 | OO | 98[A] | ALA |
| 17 | OO | 99[A] | ALA |
| 17 | OO | 100[A] | LEU |
| 17 | OO | 111[A] | PRO |
| 17 | OO | 112[A] | PRO |
| 17 | OO | 121[A] | VAL |
| 17 | OO | 125[A] | LEU |
| 17 | OO | 130[A] | LEU |
| 17 | OO | 139[A] | LEU |
| 17 | OO | 140[A] | GLY |
| 17 | OO | 142[A] | LEU |
| 17 | OO | 144[A] | THR |
| 17 | OO | 157[A] | LEU |
| 17 | OO | 158[A] | GLU |
| 17 | OO | 161[A] | ARG |
| 17 | OO | 162[A] | LYS |
| 17 | OO | 177[A] | ALA |
| 17 | OO | 183[A] | SER |
| 17 | OO | 189[A] | GLU |
| 17 | OO | 191[A] | SER |
| 17 | OO | 193[A] | LYS |
| 19 | QQ | 23 | ASN |
| 20 | RR | 22 | ILE |
| 20 | RR | 135 | LYS |
| 21 | SS | 18 | SER |
| 21 | SS | 133 | ALA |
| 24 | VV | 44 | SER |
| 27 | YY | 104 | VAL |
| 28 | ZZ | 9 | LYS |
| 28 | ZZ | 87 | LEU |
| 28 | ZZ | 89 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | ZZ | 102 | GLU |
| 29 | aa | 34 | MET |
| 29 | aa | 50 | PRO |
| 29 | aa | 78 | LEU |
| 29 | aa | 93 | SER |
| 32 | dd | 84 | ASP |
| 34 | ff | 104 | PRO |
| 35 | gg | 7 | PHE |
| 35 | gg | 56 | THR |
| 35 | gg | 60 | ARG |
| 35 | gg | 75 | ALA |
| 35 | gg | 77 | GLY |
| 35 | gg | 82 | ALA |
| 37 | ii | 13 | LYS |
| 37 | ii | 29 | ARG |
| 39 | kk | 51 | LEU |
| 40 | ll | 3 | ALA |
| 43 | oo | 6 | LYS |
| 43 | oo | 61 | LYS |
| 44 | pp | 37 | TYR |
| 44 | pp | 56 | SER |
| 44 | pp | 63 | THR |
| 45 | qq | 24 | LYS |
| 45 | qq | 119 | GLN |
| 45 | qq | 120 | VAL |
| 45 | qq | 121 | PRO |
| 45 | qq | 124 | LEU |
| 45 | qq | 172 | VAL |
| 45 | qq | 213 | ALA |
| 46 | rr | 70 | SER |
| 46 | rr | 106 | LYS |
| 46 | rr | 156 | SER |
| 48 | A | 130 | ALA |
| 48 | A | 197 | ILE |
| 49 | B | 35 | PRO |
| 49 | B | 100 | PHE |
| 50 | C | 57 | SER |
| 50 | C | 59 | GLU |
| 50 | C | 83 | ASP |
| 50 | C | 175 | ILE |
| 51 | D | 164 | VAL |
| 52 | E | 117 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | E | 129 | VAL |
| 53 | F | 59 | SER |
| 54 | G | 154 | ARG |
| 55 | H | 32 | PRO |
| 55 | H | 64 | VAL |
| 55 | H | 74 | GLN |
| 56 | I | 22 | ARG |
| 56 | I | 52 | ASN |
| 57 | J | 171 | ARG |
| 58 | K | 81 | ASN |
| 58 | K | 88 | PRO |
| 59 | L | 3 | THR |
| 59 | L | 105 | LYS |
| 59 | L | 133 | LYS |
| 62 | O | 91 | SER |
| 63 | P | 20 | VAL |
| 63 | P | 29 | PRO |
| 64 | Q | 40 | GLN |
| 65 | R | 26 | MET |
| 65 | R | 121 | VAL |
| 66 | S | 92 | VAL |
| 68 | U | 118 | ILE |
| 69 | V | 30 | SER |
| 70 | W | 57 | ARG |
| 71 | X | 4 | GLY |
| 71 | X | 12 | ALA |
| 71 | X | 42 | PRO |
| 71 | X | 63 | GLN |
| 71 | X | 64 | PRO |
| 71 | X | 131 | SER |
| 72 | Y | 30 | PRO |
| 74 | a | 10 | ARG |
| 74 | a | 18 | VAL |
| 74 | a | 75 | ILE |
| 74 | a | 81 | ALA |
| 74 | a | 86 | VAL |
| 75 | b | 21 | LEU |
| 78 | e | 11 | ALA |
| 79 | f | 111 | GLU |
| 79 | f | 143 | HIS |
| 80 | g | 293 | ASP |
| 83 | 1 | 23 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 83 | 1 | 46 | ILE |
| 83 | 1 | 162 | ARG |
| 83 | 1 | 209 | VAL |
| 83 | 1 | 247 | ASP |
| 83 | 1 | 251 | ASN |
| 83 | 1 | 305 | ILE |
| 83 | 1 | 382 | VAL |
| 83 | 1 | 406 | LYS |
| 83 | 1 | 444 | PRO |
| 83 | 1 | 548 | ASP |
| 83 | 1 | 559 | PRO |
| 83 | 1 | 578 | LYS |
| 83 | 1 | 579 | SER |
| 83 | 1 | 581 | ASN |
| 83 | 1 | 591 | GLU |
| 83 | 1 | 683 | SER |
| 83 | 1 | 691 | VAL |
| 83 | 1 | 695 | ALA |
| 83 | 1 | 702 | GLY |
| 83 | 1 | 707 | PRO |
| 83 | 1 | 721 | ASP |
| 83 | 1 | 722 | PRO |
| 83 | 1 | 727 | PRO |
| 4 | AA | 33 | ASP |
| 4 | AA | 104 | LEU |
| 4 | AA | 144 | ASN |
| 4 | AA | 154 | ALA |
| 5 | BB | 140 | ASN |
| 5 | BB | 252 | ILE |
| 5 | BB | 269 | GLN |
| 5 | BB | 317 | ILE |
| 5 | BB | 351 | LEU |
| 5 | BB | 382 | THR |
| 6 | CC | 14 | GLU |
| 6 | CC | 293 | THR |
| 6 | CC | 311 | HIS |
| 6 | CC | 341 | SER |
| 6 | CC | 342 | LYS |
| 6 | CC | 343 | LYS |
| 7 | DD | 5 | LYS |
| 7 | DD | 26 | GLY |
| 8 | EE | 115 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 8 | EE | 128 | GLU |
| 9 | FF | 104 | ARG |
| 10 | GG | 74 | ILE |
| 12 | II | 187 | ALA |
| 13 | JJ | 25 | GLU |
| 13 | JJ | 114 | ILE |
| 14 | LL | 6 | ASN |
| 14 | LL | 28 | GLN |
| 14 | LL | 190 | LYS |
| 15 | MM | 36 | VAL |
| 17 | OO | 6[A] | PRO |
| 17 | OO | 15[A] | HIS |
| 17 | OO | 16[A] | LEU |
| 17 | OO | 59[A] | LEU |
| 17 | OO | 105[A] | VAL |
| 17 | OO | 123[A] | GLN |
| 17 | OO | 146[A] | VAL |
| 17 | OO | 159[A] | GLU |
| 17 | OO | 173[A] | LYS |
| 17 | OO | 174[A] | ALA |
| 17 | OO | 187[A] | GLY |
| 17 | OO | 188[A] | THR |
| 17 | OO | 195[A] | ALA |
| 17 | OO | 198[A] | GLY |
| 18 | PP | 166 | ALA |
| 22 | TT | 12 | ARG |
| 22 | TT | 18 | ASP |
| 22 | TT | 46 | GLY |
| 22 | TT | 80 | VAL |
| 24 | VV | 21 | ALA |
| 24 | VV | 54 | LEU |
| 27 | YY | 55 | GLU |
| 28 | ZZ | 5 | LEU |
| 28 | ZZ | 59 | ALA |
| 30 | bb | 25 | LYS |
| 30 | bb | 26 | THR |
| 37 | ii | 30 | LYS |
| 43 | oo | 14 | GLY |
| 44 | pp | 47 | VAL |
| 44 | pp | 48 | LYS |
| 44 | pp | 60 | CYS |
| 45 | qq | 9 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | qq | 125 | GLY |
| 46 | rr | 38 | GLN |
| 46 | rr | 94 | SER |
| 46 | rr | 95 | LEU |
| 46 | rr | 126 | VAL |
| 48 | A | 72 | ASP |
| 48 | A | 97 | PRO |
| 48 | A | 120 | LEU |
| 50 | C | 65 | SER |
| 50 | C | 149 | TRP |
| 50 | C | 153 | LEU |
| 51 | D | 217 | VAL |
| 52 | E | 68 | ARG |
| 52 | E | 119 | ALA |
| 52 | E | 120 | SER |
| 52 | E | 186 | GLY |
| 52 | E | 201 | HIS |
| 52 | E | 205 | PHE |
| 53 | F | 166 | PRO |
| 53 | F | 206 | GLY |
| 54 | G | 122 | GLU |
| 54 | G | 156 | TYR |
| 55 | H | 10 | SER |
| 55 | H | 13 | PRO |
| 55 | H | 53 | GLY |
| 55 | H | 113 | PRO |
| 56 | I | 10 | LYS |
| 56 | I | 16 | ALA |
| 56 | I | 17 | LYS |
| 56 | I | 153 | ILE |
| 57 | J | 65 | LYS |
| 57 | J | 118 | LEU |
| 60 | M | 82 | VAL |
| 61 | N | 70 | LYS |
| 61 | N | 133 | SER |
| 64 | Q | 27 | GLY |
| 64 | Q | 116 | LEU |
| 64 | Q | 138 | PHE |
| 65 | R | 80 | ARG |
| 65 | R | 127 | VAL |
| 66 | S | 26 | ILE |
| 67 | T | 43 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 70 | W | 83 | ILE |
| 72 | Y | 61 | ARG |
| 73 | Z | 97 | LYS |
| 74 | a | 16 | GLY |
| 74 | a | 85 | ARG |
| 75 | b | 3 | LEU |
| 79 | f | 88 | PRO |
| 79 | f | 89 | LYS |
| 80 | g | 77 | ASP |
| 80 | g | 244 | LYS |
| 83 | 1 | 45 | ILE |
| 83 | 1 | 155 | VAL |
| 83 | 1 | 241 | MET |
| 83 | 1 | 245 | TRP |
| 83 | 1 | 280 | PRO |
| 83 | 1 | 497 | ASN |
| 83 | 1 | 724 | ILE |
| 4 | AA | 180 | LEU |
| 4 | AA | 201 | GLY |
| 5 | BB | 5 | LYS |
| 5 | BB | 22 | ALA |
| 5 | BB | 36 | ASP |
| 5 | BB | 173 | GLN |
| 5 | BB | 174 | LYS |
| 6 | CC | 106 | TRP |
| 6 | CC | 140 | HIS |
| 6 | CC | 201 | GLN |
| 6 | CC | 268 | ALA |
| 6 | CC | 269 | SER |
| 6 | CC | 305 | ALA |
| 6 | CC | 320 | ASN |
| 7 | DD | 259 | LYS |
| 10 | GG | 38 | ALA |
| 13 | JJ | 138 | VAL |
| 13 | JJ | 144 | CYS |
| 13 | JJ | 168 | ASP |
| 15 | MM | 5 | SER |
| 15 | MM | 29 | ALA |
| 16 | NN | 97 | SER |
| 17 | OO | 13[A] | LYS |
| 17 | OO | 48[A] | PHE |
| 17 | OO | 63[A] | THR |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 17 | OO | 114[A] | ASP |
| 17 | OO | 143[A] | SER |
| 17 | OO | 167[A] | GLU |
| 18 | PP | 17 | ALA |
| 18 | PP | 161 | SER |
| 19 | QQ | 183 | ALA |
| 20 | RR | 129 | GLY |
| 21 | SS | 13 | ARG |
| 21 | SS | 24 | LEU |
| 22 | TT | 47 | SER |
| 27 | YY | 103 | LYS |
| 28 | ZZ | 70 | PRO |
| 29 | aa | 48 | TYR |
| 35 | gg | 57 | LEU |
| 37 | ii | 28 | TYR |
| 39 | kk | 6 | ALA |
| 39 | kk | 40 | GLN |
| 45 | qq | 71 | ALA |
| 45 | qq | 113 | SER |
| 45 | qq | 129 | SER |
| 45 | qq | 209 | THR |
| 46 | rr | 28 | PHE |
| 46 | rr | 68 | PHE |
| 46 | rr | 69 | ILE |
| 46 | rr | 111 | ALA |
| 46 | rr | 197 | GLN |
| 48 | A | 94 | GLY |
| 48 | A | 195 | TRP |
| 49 | B | 209 | ASN |
| 49 | B | 223 | PHE |
| 50 | C | 151 | THR |
| 51 | D | 44 | THR |
| 51 | D | 163 | PRO |
| 51 | D | 178 | ARG |
| 52 | E | 77 | ARG |
| 52 | E | 127 | LYS |
| 52 | E | 195 | ILE |
| 53 | F | 77 | GLY |
| 53 | F | 83 | ARG |
| 55 | H | 132 | PRO |
| 60 | M | 78 | PRO |
| 63 | P | 12 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 64 | Q | 14 | LYS |
| 65 | R | 100 | LEU |
| 69 | V | 4 | ASP |
| 69 | V | 44 | ARG |
| 70 | W | 78 | ARG |
| 71 | X | 47 | SER |
| 72 | Y | 64 | TYR |
| 74 | a | 12 | LYS |
| 74 | a | 20 | PRO |
| 74 | a | 33 | ASP |
| 74 | a | 49 | ALA |
| 74 | a | 51 | ARG |
| 74 | a | 84 | VAL |
| 78 | e | 61 | SER |
| 79 | f | 97 | LYS |
| 80 | g | 4 | SER |
| 80 | g | 52 | GLU |
| 80 | g | 54 | GLN |
| 83 | 1 | 29 | ASP |
| 83 | 1 | 379 | MET |
| 83 | 1 | 653 | VAL |
| 4 | AA | 103 | PRO |
| 5 | BB | 227 | GLU |
| 6 | CC | 131 | VAL |
| 6 | CC | 338 | LYS |
| 6 | CC | 351 | PRO |
| 7 | DD | 21 | ARG |
| 7 | DD | 44 | TYR |
| 10 | GG | 24 | PRO |
| 10 | GG | 32 | ASN |
| 13 | JJ | 10 | ARG |
| 14 | LL | 4 | SER |
| 14 | LL | 155 | GLU |
| 15 | MM | 6 | VAL |
| 16 | NN | 81 | TYR |
| 17 | OO | 39[A] | ALA |
| 17 | OO | 77[A] | PRO |
| 17 | OO | 83[A] | LYS |
| 17 | OO | 175[A] | TYR |
| 21 | SS | 167 | ARG |
| 22 | TT | 146 | ASN |
| 24 | VV | 82 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | XX | 64 | GLU |
| 29 | aa | 124 | ILE |
| 32 | dd | 15 | ASN |
| 32 | dd | 28 | ARG |
| 32 | dd | 82 | GLU |
| 33 | ee | 123 | LYS |
| 36 | hh | 84 | LYS |
| 36 | hh | 85 | THR |
| 37 | ii | 63 | ASN |
| 38 | jj | 20 | LYS |
| 40 | ll | 20 | ASN |
| 41 | mm | 79 | GLU |
| 44 | pp | 57 | CYS |
| 44 | pp | 61 | ASN |
| 45 | qq | 61 | PRO |
| 46 | rr | 189 | VAL |
| 48 | A | 26 | ALA |
| 48 | A | 103 | THR |
| 48 | A | 167 | LYS |
| 48 | A | 193 | GLN |
| 49 | B | 210 | VAL |
| 50 | C | 41 | VAL |
| 51 | D | 93 | ASP |
| 52 | E | 223 | ASN |
| 54 | G | 165 | GLY |
| 55 | H | 111 | LYS |
| 57 | J | 67 | PRO |
| 57 | J | 69 | ARG |
| 57 | J | 147 | MET |
| 59 | L | 30 | LYS |
| 59 | L | 55 | ASP |
| 62 | O | 18 | ARG |
| 63 | P | 101 | VAL |
| 64 | Q | 115 | THR |
| 66 | S | 12 | GLN |
| 67 | T | 50 | SER |
| 68 | U | 71 | PRO |
| 69 | V | 22 | ARG |
| 71 | X | 24 | TRP |
| 71 | X | 89 | ASN |
| 73 | Z | 58 | ARG |
| 74 | a | 8 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 80 | g | 288 | TYR |
| 83 | 1 | 208 | THR |
| 83 | 1 | 246 | GLY |
| 83 | 1 | 589 | LYS |
| 83 | 1 | 675 | PRO |
| 83 | 1 | 681 | MET |
| 83 | 1 | 795 | GLN |
| 4 | AA | 56 | ALA |
| 5 | BB | 155 | ALA |
| 5 | BB | 383 | LEU |
| 6 | CC | 317 | PRO |
| 7 | DD | 6 | ASP |
| 7 | DD | 258 | LYS |
| 7 | DD | 276 | LYS |
| 8 | EE | 8 | TYR |
| 9 | FF | 205 | SER |
| 11 | HH | 110 | LYS |
| 14 | LL | 130 | GLY |
| 15 | MM | 41 | GLN |
| 17 | OO | 38[A] | ARG |
| 18 | PP | 158 | GLU |
| 18 | PP | 165 | VAL |
| 19 | QQ | 168 | THR |
| 19 | QQ | 179 | ARG |
| 20 | RR | 53 | LYS |
| 22 | TT | 127 | GLN |
| 24 | VV | 53 | SER |
| 28 | ZZ | 19 | ALA |
| 29 | aa | 49 | HIS |
| 36 | hh | 86 | ARG |
| 44 | pp | 51 | ALA |
| 45 | qq | 7 | SER |
| 45 | qq | 25 | LYS |
| 46 | rr | 80 | PRO |
| 46 | rr | 149 | ARG |
| 48 | A | 28 | ASN |
| 49 | B | 145 | LYS |
| 50 | C | 226 | THR |
| 53 | F | 82 | LYS |
| 54 | G | 173 | PRO |
| 54 | G | 177 | ARG |
| 55 | H | 134 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 56 | I | 40 | THR |
| 57 | J | 18 | PRO |
| 57 | J | 134 | ILE |
| 58 | K | 83 | PRO |
| 63 | P | 69 | GLU |
| 63 | P | 121 | ILE |
| 66 | S | 14 | ILE |
| 68 | U | 21 | LYS |
| 72 | Y | 36 | SER |
| 72 | Y | 63 | GLN |
| 73 | Z | 73 | GLY |
| 74 | a | 83 | ILE |
| 75 | b | 62 | VAL |
| 80 | g | 139 | GLY |
| 80 | g | 168 | ASP |
| 83 | 1 | 44 | GLY |
| 83 | 1 | 792 | ALA |
| 6 | CC | 78 | GLY |
| 7 | DD | 7 | ILE |
| 7 | DD | 125 | VAL |
| 13 | JJ | 108 | GLU |
| 17 | OO | 160[A] | LYS |
| 18 | PP | 160 | ALA |
| 20 | RR | 130 | ASN |
| 22 | TT | 69 | LYS |
| 43 | oo | 95 | GLY |
| 50 | C | 44 | THR |
| 53 | F | 221 | ARG |
| 54 | G | 8 | PRO |
| 57 | J | 120 | LYS |
| 58 | K | 94 | GLY |
| 59 | L | 4 | GLU |
| 63 | P | 28 | MET |
| 71 | X | 130 | VAL |
| 72 | Y | 29 | HIS |
| 72 | Y | 51 | GLU |
| 72 | Y | 66 | GLY |
| 74 | a | 82 | ARG |
| 78 | e | 47 | VAL |
| 80 | g | 75 | SER |
| 83 | 1 | 372 | CYS |
| 83 | 1 | 374 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 83 | 1 | 481 | MET |
| 83 | 1 | 486 | SER |
| 83 | 1 | 487 | PRO |
| 5 | BB | 223 | GLY |
| 7 | DD | 4 | ILE |
| 9 | FF | 175 | ILE |
| 9 | FF | 213 | VAL |
| 17 | OO | 85[A] | VAL |
| 35 | gg | 59 | PRO |
| 46 | rr | 133 | GLY |
| 69 | V | 82 | VAL |
| 83 | 1 | 580 | PRO |
| 13 | JJ | 65 | ILE |
| 17 | OO | 71[A] | PRO |
| 32 | dd | 66 | GLY |
| 55 | H | 8 | ILE |
| 59 | L | 7 | VAL |
| 60 | M | 97 | ILE |
| 66 | S | 76 | PRO |
| 70 | W | 29 | PRO |
| 71 | X | 53 | VAL |
| 75 | b | 39 | GLY |
| 83 | 1 | 558 | PRO |
| 83 | 1 | 827 | GLY |
| 12 | II | 93 | PRO |
| 18 | PP | 117 | ILE |
| 20 | RR | 94 | VAL |
| 48 | A | 158 | VAL |
| 49 | B | 206 | PRO |
| 51 | D | 130 | GLY |
| 54 | G | 70 | PRO |
| 60 | M | 48 | GLY |
| 64 | Q | 39 | VAL |
| 74 | a | 36 | ILE |
| 79 | f | 102 | VAL |
| 80 | g | 138 | VAL |
| 9 | FF | 188 | VAL |
| 10 | GG | 35 | ILE |
| 17 | OO | 76[A] | ALA |
| 55 | H | 98 | ILE |
| 62 | O | 118 | VAL |
| 83 | 1 | 808 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57 | J | 162 | SER |
| 70 | W | 76 | SER |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4 | AA | 190/190 (100%) | 174 (92%) | 16 (8%) | 13 | 49 |
| 5 | BB | 323/323 (100%) | 272 (84%) | 51 (16%) | 3 | 21 |
| 6 | CC | 288/291 (99%) | 253 (88%) | 35 (12%) | 6 | 31 |
| 7 | DD | 243/243 (100%) | 215 (88%) | 28 (12%) | 6 | 35 |
| 8 | EE | 139/147 (95%) | 128 (92%) | 11 (8%) | 14 | 51 |
| 9 | FF | 188/188 (100%) | 167 (89%) | 21 (11%) | 7 | 36 |
| 10 | GG | 192/194 (99%) | 175 (91%) | 17 (9%) | 11 | 46 |
| 11 | HH | 173/173 (100%) | 155 (90%) | 18 (10%) | 8 | 39 |
| 12 | II | 177/185 (96%) | 156 (88%) | 21 (12%) | 6 | 33 |
| 13 | JJ | 144/144 (100%) | 130 (90%) | 14 (10%) | 9 | 42 |
| 14 | LL | 162/162 (100%) | 149 (92%) | 13 (8%) | 14 | 50 |
| 15 | MM | 109/109 (100%) | 93 (85%) | 16 (15%) | 3 | 24 |
| 16 | NN | 175/175 (100%) | 156 (89%) | 19 (11%) | 7 | 37 |
| 17 | OO | 163/163 (100%) | 136 (83%) | 27 (17%) | 2 | 18 |
| 18 | PP | 148/148 (100%) | 132 (89%) | 16 (11%) | 7 | 38 |
| 19 | QQ | 150/150 (100%) | 139 (93%) | 11 (7%) | 16 | 54 |
| 20 | RR | 152/152 (100%) | 147 (97%) | 5 (3%) | 43 | 77 |
| 21 | SS | 154/154 (100%) | 145 (94%) | 9 (6%) | 23 | 62 |
| 22 | TT | 135/135 (100%) | 118 (87%) | 17 (13%) | 5 | 30 |
| 23 | UU | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 24 | VV | 101/101 (100%) | 90 (89%) | 11 (11%) | 7 | 37 |
| 25 | WW | 54/54 (100%) | 52 (96%) | 2 (4%) | 39 | 74 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 26 | XX | 106/106 (100%) | 91 (86%) | 15 (14%) | 4 | 26 |
| 27 | YY | 111/111 (100%) | 102 (92%) | 9 (8%) | 14 | 50 |
| 28 | ZZ | 115/115 (100%) | 106 (92%) | 9 (8%) | 15 | 51 |
| 29 | aa | 117/117 (100%) | 104 (89%) | 13 (11%) | 7 | 37 |
| 30 | bb | 45/45 (100%) | 44 (98%) | 1 (2%) | 57 | 84 |
| 31 | cc | 79/79 (100%) | 72 (91%) | 7 (9%) | 11 | 46 |
| 32 | dd | 95/95 (100%) | 88 (93%) | 7 (7%) | 16 | 53 |
| 33 | ee | 106/106 (100%) | 100 (94%) | 6 (6%) | 24 | 63 |
| 34 | ff | 90/90 (100%) | 84 (93%) | 6 (7%) | 19 | 58 |
| 35 | gg | 102/102 (100%) | 100 (98%) | 2 (2%) | 60 | 85 |
| 36 | hh | 104/104 (100%) | 100 (96%) | 4 (4%) | 38 | 74 |
| 37 | ii | 79/79 (100%) | 70 (89%) | 9 (11%) | 7 | 35 |
| 38 | jj | 69/69 (100%) | 61 (88%) | 8 (12%) | 6 | 34 |
| 39 | kk | 68/68 (100%) | 63 (93%) | 5 (7%) | 16 | 53 |
| 40 | ll | 44/44 (100%) | 41 (93%) | 3 (7%) | 18 | 57 |
| 41 | mm | 46/46 (100%) | 42 (91%) | 4 (9%) | 12 | 47 |
| 42 | nn | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 15 |
| 43 | oo | 86/86 (100%) | 76 (88%) | 10 (12%) | 6 | 34 |
| 44 | pp | 69/69 (100%) | 58 (84%) | 11 (16%) | 3 | 20 |
| 45 | qq | 198/198 (100%) | 181 (91%) | 17 (9%) | 12 | 48 |
| 46 | rr | 162/162 (100%) | 147 (91%) | 15 (9%) | 10 | 45 |
| 48 | A | 174/174 (100%) | 159 (91%) | 15 (9%) | 12 | 48 |
| 49 | B | 196/196 (100%) | 178 (91%) | 18 (9%) | 11 | 45 |
| 50 | C | 176/176 (100%) | 152 (86%) | 24 (14%) | 4 | 28 |
| 51 | D | 185/185 (100%) | 165 (89%) | 20 (11%) | 7 | 38 |
| 52 | E | 223/223 (100%) | 199 (89%) | 24 (11%) | 7 | 38 |
| 53 | F | 174/174 (100%) | 165 (95%) | 9 (5%) | 27 | 65 |
| 54 | G | 192/192 (100%) | 179 (93%) | 13 (7%) | 18 | 57 |
| 55 | H | 164/164 (100%) | 152 (93%) | 12 (7%) | 16 | 54 |
| 56 | I | 148/158 (94%) | 131 (88%) | 17 (12%) | 6 | 35 |
| 57 | J | 153/153 (100%) | 137 (90%) | 16 (10%) | 8 | 39 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|------------|------------|-------------|----|
| 58 | K | 88/88 (100%) | 81 (92%) | 7 (8%) | 14 | 50 |
| 59 | L | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 43 |
| 60 | M | 97/97 (100%) | 92 (95%) | 5 (5%) | 27 | 65 |
| 61 | N | 127/127 (100%) | 112 (88%) | 15 (12%) | 6 | 33 |
| 62 | O | 96/96 (100%) | 87 (91%) | 9 (9%) | 10 | 44 |
| 63 | P | 105/105 (100%) | 92 (88%) | 13 (12%) | 5 | 31 |
| 64 | Q | 117/117 (100%) | 111 (95%) | 6 (5%) | 28 | 66 |
| 65 | R | 117/117 (100%) | 107 (92%) | 10 (8%) | 12 | 48 |
| 66 | S | 128/128 (100%) | 112 (88%) | 16 (12%) | 5 | 31 |
| 67 | T | 117/117 (100%) | 110 (94%) | 7 (6%) | 22 | 62 |
| 68 | U | 96/96 (100%) | 92 (96%) | 4 (4%) | 34 | 71 |
| 69 | V | 73/73 (100%) | 65 (89%) | 8 (11%) | 7 | 37 |
| 70 | W | 110/110 (100%) | 94 (86%) | 16 (14%) | 4 | 25 |
| 71 | X | 120/120 (100%) | 107 (89%) | 13 (11%) | 7 | 38 |
| 72 | Y | 108/108 (100%) | 99 (92%) | 9 (8%) | 13 | 49 |
| 73 | Z | 60/60 (100%) | 57 (95%) | 3 (5%) | 28 | 66 |
| 74 | a | 85/85 (100%) | 73 (86%) | 12 (14%) | 4 | 26 |
| 75 | b | 72/72 (100%) | 68 (94%) | 4 (6%) | 25 | 63 |
| 76 | c | 55/55 (100%) | 52 (94%) | 3 (6%) | 25 | 64 |
| 77 | d | 46/46 (100%) | 43 (94%) | 3 (6%) | 20 | 59 |
| 78 | e | 49/49 (100%) | 46 (94%) | 3 (6%) | 22 | 61 |
| 79 | f | 58/60 (97%) | 48 (83%) | 10 (17%) | 2 | 16 |
| 80 | g | 265/270 (98%) | 246 (93%) | 19 (7%) | 17 | 55 |
| 83 | 1 | 700/702 (100%) | 612 (87%) | 88 (13%) | 5 | 30 |
| All | All | 10374/10414 (100%) | 9367 (90%) | 1007 (10%) | 14 | 42 |

All (1007) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AA | 21 | ARG |
| 4 | AA | 32 | LEU |
| 4 | AA | 51 | ASP |
| 4 | AA | 92 | LYS |
| 4 | AA | 96 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AA | 123 | ARG |
| 4 | AA | 126 | LEU |
| 4 | AA | 130 | SER |
| 4 | AA | 143 | ASP |
| 4 | AA | 161 | ASP |
| 4 | AA | 180 | LEU |
| 4 | AA | 190 | ARG |
| 4 | AA | 193 | ARG |
| 4 | AA | 204 | MET |
| 4 | AA | 241 | ARG |
| 4 | AA | 243 | THR |
| 5 | BB | 4 | ARG |
| 5 | BB | 7 | GLU |
| 5 | BB | 10 | ARG |
| 5 | BB | 14 | LEU |
| 5 | BB | 21 | ARG |
| 5 | BB | 45 | SER |
| 5 | BB | 54 | SER |
| 5 | BB | 56 | ILE |
| 5 | BB | 58 | ARG |
| 5 | BB | 59 | ASP |
| 5 | BB | 60 | LEU |
| 5 | BB | 80 | ASP |
| 5 | BB | 84 | ILE |
| 5 | BB | 87 | VAL |
| 5 | BB | 100 | ARG |
| 5 | BB | 101 | SER |
| 5 | BB | 102 | LEU |
| 5 | BB | 103 | THR |
| 5 | BB | 117 | ARG |
| 5 | BB | 121 | ASN |
| 5 | BB | 125 | SER |
| 5 | BB | 128 | LYS |
| 5 | BB | 162 | VAL |
| 5 | BB | 164 | THR |
| 5 | BB | 169 | THR |
| 5 | BB | 187 | SER |
| 5 | BB | 193 | ASP |
| 5 | BB | 241 | LYS |
| 5 | BB | 255 | TRP |
| 5 | BB | 262 | TRP |
| 5 | BB | 266 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | BB | 272 | TYR |
| 5 | BB | 274 | HIS |
| 5 | BB | 289 | ASP |
| 5 | BB | 290 | ASP |
| 5 | BB | 304 | THR |
| 5 | BB | 305 | ILE |
| 5 | BB | 306 | THR |
| 5 | BB | 323 | ILE |
| 5 | BB | 324 | LEU |
| 5 | BB | 325 | LYS |
| 5 | BB | 328 | ILE |
| 5 | BB | 331 | THR |
| 5 | BB | 332 | ARG |
| 5 | BB | 336 | VAL |
| 5 | BB | 339 | ARG |
| 5 | BB | 355 | THR |
| 5 | BB | 369 | ARG |
| 5 | BB | 370 | PHE |
| 5 | BB | 382 | THR |
| 5 | BB | 384 | LYS |
| 6 | CC | 19 | ASP |
| 6 | CC | 31 | ARG |
| 6 | CC | 37 | SER |
| 6 | CC | 41 | SER |
| 6 | CC | 58 | HIS |
| 6 | CC | 85 | SER |
| 6 | CC | 92 | ASN |
| 6 | CC | 93 | MET |
| 6 | CC | 95 | ARG |
| 6 | CC | 98 | ARG |
| 6 | CC | 105 | THR |
| 6 | CC | 107 | ARG |
| 6 | CC | 120 | TYR |
| 6 | CC | 122 | THR |
| 6 | CC | 134 | LEU |
| 6 | CC | 138 | ARG |
| 6 | CC | 156 | LEU |
| 6 | CC | 157 | GLN |
| 6 | CC | 175 | HIS |
| 6 | CC | 177 | ASP |
| 6 | CC | 180 | LYS |
| 6 | CC | 182 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CC | 194 | TYR |
| 6 | CC | 198 | ARG |
| 6 | CC | 202 | ARG |
| 6 | CC | 206 | LEU |
| 6 | CC | 215 | VAL |
| 6 | CC | 232 | SER |
| 6 | CC | 235 | LEU |
| 6 | CC | 238 | LEU |
| 6 | CC | 247 | PHE |
| 6 | CC | 270 | VAL |
| 6 | CC | 346 | GLN |
| 6 | CC | 350 | LYS |
| 6 | CC | 356 | LEU |
| 7 | DD | 4 | ILE |
| 7 | DD | 22 | ARG |
| 7 | DD | 28 | THR |
| 7 | DD | 51 | LEU |
| 7 | DD | 54 | ARG |
| 7 | DD | 59 | ASP |
| 7 | DD | 67 | SER |
| 7 | DD | 70 | THR |
| 7 | DD | 75 | LEU |
| 7 | DD | 89 | THR |
| 7 | DD | 94 | ASN |
| 7 | DD | 101 | THR |
| 7 | DD | 103 | LEU |
| 7 | DD | 116 | ASP |
| 7 | DD | 144 | VAL |
| 7 | DD | 147 | ASP |
| 7 | DD | 152 | ARG |
| 7 | DD | 154 | THR |
| 7 | DD | 155 | THR |
| 7 | DD | 179 | ARG |
| 7 | DD | 184 | ASP |
| 7 | DD | 193 | ASP |
| 7 | DD | 195 | LEU |
| 7 | DD | 213 | ASP |
| 7 | DD | 214 | ASP |
| 7 | DD | 230 | ASP |
| 7 | DD | 278 | THR |
| 7 | DD | 293 | LEU |
| 8 | EE | 29 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | EE | 48 | LYS |
| 8 | EE | 50 | VAL |
| 8 | EE | 74 | LEU |
| 8 | EE | 76 | ARG |
| 8 | EE | 82 | VAL |
| 8 | EE | 111 | ARG |
| 8 | EE | 114 | ARG |
| 8 | EE | 126 | LYS |
| 8 | EE | 154 | LEU |
| 8 | EE | 174 | LYS |
| 9 | FF | 30 | ARG |
| 9 | FF | 53 | GLU |
| 9 | FF | 57 | ARG |
| 9 | FF | 70 | SER |
| 9 | FF | 71 | SER |
| 9 | FF | 75 | SER |
| 9 | FF | 81 | VAL |
| 9 | FF | 85 | ARG |
| 9 | FF | 87 | LYS |
| 9 | FF | 90 | ASN |
| 9 | FF | 110 | SER |
| 9 | FF | 112 | THR |
| 9 | FF | 140 | THR |
| 9 | FF | 156 | GLN |
| 9 | FF | 181 | LEU |
| 9 | FF | 218 | LYS |
| 9 | FF | 221 | ILE |
| 9 | FF | 225 | SER |
| 9 | FF | 226 | PHE |
| 9 | FF | 233 | ILE |
| 9 | FF | 236 | LEU |
| 10 | GG | 28 | SER |
| 10 | GG | 62 | LYS |
| 10 | GG | 70 | VAL |
| 10 | GG | 123 | GLU |
| 10 | GG | 130 | VAL |
| 10 | GG | 135 | LEU |
| 10 | GG | 144 | ASN |
| 10 | GG | 154 | ASN |
| 10 | GG | 155 | ASP |
| 10 | GG | 165 | LEU |
| 10 | GG | 168 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | GG | 184 | ARG |
| 10 | GG | 196 | VAL |
| 10 | GG | 220 | ASN |
| 10 | GG | 222 | LEU |
| 10 | GG | 231 | HIS |
| 10 | GG | 240 | LYS |
| 11 | HH | 5 | GLN |
| 11 | HH | 11 | ASP |
| 11 | HH | 41 | ILE |
| 11 | HH | 42 | ASP |
| 11 | HH | 69 | ARG |
| 11 | HH | 80 | THR |
| 11 | HH | 83 | THR |
| 11 | HH | 91 | ARG |
| 11 | HH | 118 | LEU |
| 11 | HH | 120 | ASP |
| 11 | HH | 143 | GLU |
| 11 | HH | 157 | ASN |
| 11 | HH | 168 | ARG |
| 11 | HH | 170 | LYS |
| 11 | HH | 172 | ILE |
| 11 | HH | 173 | ARG |
| 11 | HH | 186 | LEU |
| 11 | HH | 189 | GLU |
| 12 | II | 7 | ARG |
| 12 | II | 24 | ARG |
| 12 | II | 30 | LYS |
| 12 | II | 33 | ILE |
| 12 | II | 40 | LYS |
| 12 | II | 52 | LEU |
| 12 | II | 57 | LEU |
| 12 | II | 88 | ARG |
| 12 | II | 90 | ARG |
| 12 | II | 91 | VAL |
| 12 | II | 115 | MET |
| 12 | II | 140 | THR |
| 12 | II | 142 | ASP |
| 12 | II | 144 | ASN |
| 12 | II | 154 | ARG |
| 12 | II | 163 | GLN |
| 12 | II | 165 | ILE |
| 12 | II | 169 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | II | 193 | ASP |
| 12 | II | 200 | LEU |
| 12 | II | 203 | LYS |
| 13 | JJ | 12 | LEU |
| 13 | JJ | 17 | LEU |
| 13 | JJ | 30 | LEU |
| 13 | JJ | 39 | GLN |
| 13 | JJ | 44 | THR |
| 13 | JJ | 56 | THR |
| 13 | JJ | 80 | LEU |
| 13 | JJ | 92 | ARG |
| 13 | JJ | 99 | THR |
| 13 | JJ | 106 | ILE |
| 13 | JJ | 112 | LEU |
| 13 | JJ | 130 | VAL |
| 13 | JJ | 137 | ARG |
| 13 | JJ | 154 | THR |
| 14 | LL | 5 | LYS |
| 14 | LL | 24 | VAL |
| 14 | LL | 31 | LYS |
| 14 | LL | 42 | LYS |
| 14 | LL | 49 | ARG |
| 14 | LL | 54 | LEU |
| 14 | LL | 55 | ARG |
| 14 | LL | 67 | ARG |
| 14 | LL | 69 | VAL |
| 14 | LL | 110 | ASP |
| 14 | LL | 120 | GLN |
| 14 | LL | 124 | ILE |
| 14 | LL | 194 | GLU |
| 15 | MM | 2 | SER |
| 15 | MM | 5 | SER |
| 15 | MM | 8 | LYS |
| 15 | MM | 20 | VAL |
| 15 | MM | 21 | VAL |
| 15 | MM | 22 | LEU |
| 15 | MM | 34 | THR |
| 15 | MM | 53 | VAL |
| 15 | MM | 63 | VAL |
| 15 | MM | 64 | VAL |
| 15 | MM | 69 | THR |
| 15 | MM | 74 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 15 | MM | 77 | LYS |
| 15 | MM | 106 | ARG |
| 15 | MM | 121 | LEU |
| 15 | MM | 125 | LYS |
| 16 | NN | 10 | LEU |
| 16 | NN | 19 | LEU |
| 16 | NN | 22 | LEU |
| 16 | NN | 38 | ARG |
| 16 | NN | 41 | ARG |
| 16 | NN | 62 | TYR |
| 16 | NN | 80 | THR |
| 16 | NN | 83 | LYS |
| 16 | NN | 97 | SER |
| 16 | NN | 98 | LEU |
| 16 | NN | 109 | ARG |
| 16 | NN | 126 | THR |
| 16 | NN | 131 | GLU |
| 16 | NN | 133 | ILE |
| 16 | NN | 134 | LEU |
| 16 | NN | 136 | ASP |
| 16 | NN | 151 | ILE |
| 16 | NN | 183 | THR |
| 16 | NN | 196 | THR |
| 17 | OO | 5[A] | GLU |
| 17 | OO | 20[A] | LEU |
| 17 | OO | 23[A] | THR |
| 17 | OO | 32[A] | GLN |
| 17 | OO | 33[A] | LYS |
| 17 | OO | 34[A] | ILE |
| 17 | OO | 38[A] | ARG |
| 17 | OO | 42[A] | LEU |
| 17 | OO | 43[A] | ASN |
| 17 | OO | 47[A] | GLU |
| 17 | OO | 60[A] | ARG |
| 17 | OO | 69[A] | ARG |
| 17 | OO | 78[A] | SER |
| 17 | OO | 81[A] | PHE |
| 17 | OO | 82[A] | TYR |
| 17 | OO | 107[A] | GLU |
| 17 | OO | 114[A] | ASP |
| 17 | OO | 116[A] | LYS |
| 17 | OO | 117[A] | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 17 | OO | 118[A] | ARG |
| 17 | OO | 119[A] | VAL |
| 17 | OO | 125[A] | LEU |
| 17 | OO | 127[A] | VAL |
| 17 | OO | 130[A] | LEU |
| 17 | OO | 150[A] | TYR |
| 17 | OO | 152[A] | ASP |
| 17 | OO | 168[A] | TYR |
| 18 | PP | 24 | VAL |
| 18 | PP | 26 | TYR |
| 18 | PP | 52 | LEU |
| 18 | PP | 55 | GLN |
| 18 | PP | 118 | GLN |
| 18 | PP | 119 | VAL |
| 18 | PP | 120 | ASN |
| 18 | PP | 142 | SER |
| 18 | PP | 144 | SER |
| 18 | PP | 145 | HIS |
| 18 | PP | 153 | LYS |
| 18 | PP | 161 | SER |
| 18 | PP | 164 | LYS |
| 18 | PP | 168 | LEU |
| 18 | PP | 171 | ARG |
| 18 | PP | 173 | ARG |
| 19 | QQ | 17 | THR |
| 19 | QQ | 32 | LEU |
| 19 | QQ | 41 | ASP |
| 19 | QQ | 49 | LEU |
| 19 | QQ | 95 | GLU |
| 19 | QQ | 105 | ARG |
| 19 | QQ | 135 | GLN |
| 19 | QQ | 144 | ARG |
| 19 | QQ | 148 | GLU |
| 19 | QQ | 165 | ILE |
| 19 | QQ | 168 | THR |
| 20 | RR | 60 | ARG |
| 20 | RR | 91 | SER |
| 20 | RR | 99 | LEU |
| 20 | RR | 119 | LEU |
| 20 | RR | 128 | LYS |
| 21 | SS | 40 | ARG |
| 21 | SS | 45 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | SS | 52 | LYS |
| 21 | SS | 97 | VAL |
| 21 | SS | 117 | ARG |
| 21 | SS | 122 | HIS |
| 21 | SS | 137 | ARG |
| 21 | SS | 171 | PHE |
| 21 | SS | 172 | TYR |
| 22 | TT | 18 | ASP |
| 22 | TT | 41 | ASP |
| 22 | TT | 55 | LYS |
| 22 | TT | 72 | VAL |
| 22 | TT | 75 | ILE |
| 22 | TT | 78 | LYS |
| 22 | TT | 79 | MET |
| 22 | TT | 83 | ARG |
| 22 | TT | 88 | ARG |
| 22 | TT | 93 | VAL |
| 22 | TT | 97 | LYS |
| 22 | TT | 126 | VAL |
| 22 | TT | 127 | GLN |
| 22 | TT | 128 | LEU |
| 22 | TT | 139 | ARG |
| 22 | TT | 148 | PRO |
| 22 | TT | 157 | GLU |
| 24 | VV | 11 | PHE |
| 24 | VV | 33 | ASN |
| 24 | VV | 47 | ASN |
| 24 | VV | 48 | ARG |
| 24 | VV | 56 | ASP |
| 24 | VV | 63 | LYS |
| 24 | VV | 64 | LYS |
| 24 | VV | 83 | LYS |
| 24 | VV | 98 | ASN |
| 24 | VV | 102 | ILE |
| 24 | VV | 131 | SER |
| 25 | WW | 42 | GLN |
| 25 | WW | 58 | HIS |
| 26 | XX | 26 | VAL |
| 26 | XX | 27 | ARG |
| 26 | XX | 31 | SER |
| 26 | XX | 36 | LYS |
| 26 | XX | 45 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | XX | 56 | ARG |
| 26 | XX | 63 | ILE |
| 26 | XX | 68 | THR |
| 26 | XX | 73 | MET |
| 26 | XX | 82 | LEU |
| 26 | XX | 115 | ARG |
| 26 | XX | 133 | LEU |
| 26 | XX | 135 | ILE |
| 26 | XX | 137 | ASN |
| 26 | XX | 142 | ILE |
| 27 | YY | 9 | SER |
| 27 | YY | 50 | ILE |
| 27 | YY | 54 | ASP |
| 27 | YY | 55 | GLU |
| 27 | YY | 74 | TYR |
| 27 | YY | 95 | VAL |
| 27 | YY | 104 | VAL |
| 27 | YY | 112 | ASP |
| 27 | YY | 126 | LEU |
| 28 | ZZ | 34 | LYS |
| 28 | ZZ | 46 | ILE |
| 28 | ZZ | 51 | LEU |
| 28 | ZZ | 56 | ARG |
| 28 | ZZ | 57 | GLN |
| 28 | ZZ | 72 | ILE |
| 28 | ZZ | 89 | VAL |
| 28 | ZZ | 109 | GLU |
| 28 | ZZ | 121 | ARG |
| 29 | aa | 4 | ARG |
| 29 | aa | 5 | LEU |
| 29 | aa | 16 | SER |
| 29 | aa | 27 | LYS |
| 29 | aa | 43 | THR |
| 29 | aa | 44 | ASN |
| 29 | aa | 60 | TYR |
| 29 | aa | 65 | GLN |
| 29 | aa | 76 | ASP |
| 29 | aa | 115 | LYS |
| 29 | aa | 120 | ASP |
| 29 | aa | 128 | ARG |
| 29 | aa | 130 | VAL |
| 30 | bb | 32 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | cc | 16 | LEU |
| 31 | cc | 41 | LEU |
| 31 | cc | 54 | SER |
| 31 | cc | 61 | MET |
| 31 | cc | 66 | LYS |
| 31 | cc | 83 | LYS |
| 31 | cc | 93 | LEU |
| 32 | dd | 5 | LYS |
| 32 | dd | 8 | VAL |
| 32 | dd | 52 | ASP |
| 32 | dd | 55 | LEU |
| 32 | dd | 64 | ILE |
| 32 | dd | 76 | SER |
| 32 | dd | 105 | HIS |
| 33 | ee | 6 | HIS |
| 33 | ee | 19 | ARG |
| 33 | ee | 23 | ASP |
| 33 | ee | 33 | ARG |
| 33 | ee | 50 | ILE |
| 33 | ee | 75 | LEU |
| 34 | ff | 17 | GLN |
| 34 | ff | 20 | LYS |
| 34 | ff | 33 | GLU |
| 34 | ff | 77 | ASN |
| 34 | ff | 81 | VAL |
| 34 | ff | 105 | SER |
| 35 | gg | 60 | ARG |
| 35 | gg | 62 | TYR |
| 36 | hh | 69 | LEU |
| 36 | hh | 81 | ARG |
| 36 | hh | 85 | THR |
| 36 | hh | 102 | GLU |
| 37 | ii | 18 | ASN |
| 37 | ii | 34 | SER |
| 37 | ii | 57 | LEU |
| 37 | ii | 58 | ILE |
| 37 | ii | 62 | ARG |
| 37 | ii | 75 | LYS |
| 37 | ii | 76 | ARG |
| 37 | ii | 84 | LYS |
| 37 | ii | 99 | ARG |
| 38 | jj | 5 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | jj | 7 | SER |
| 38 | jj | 15 | SER |
| 38 | jj | 17 | THR |
| 38 | jj | 24 | ARG |
| 38 | jj | 45 | ARG |
| 38 | jj | 59 | THR |
| 38 | jj | 75 | LYS |
| 39 | kk | 8 | ILE |
| 39 | kk | 32 | ASN |
| 39 | kk | 51 | LEU |
| 39 | kk | 53 | THR |
| 39 | kk | 73 | PHE |
| 40 | ll | 6 | SER |
| 40 | ll | 21 | ARG |
| 40 | ll | 29 | LEU |
| 41 | mm | 85 | LEU |
| 41 | mm | 97 | ARG |
| 41 | mm | 106 | ARG |
| 41 | mm | 113 | ARG |
| 42 | nn | 2 | ARG |
| 42 | nn | 6 | ARG |
| 42 | nn | 13 | LEU |
| 42 | nn | 16 | LYS |
| 43 | oo | 12 | CYS |
| 43 | oo | 29 | LYS |
| 43 | oo | 45 | ARG |
| 43 | oo | 47 | GLN |
| 43 | oo | 48 | SER |
| 43 | oo | 61 | LYS |
| 43 | oo | 78 | LYS |
| 43 | oo | 83 | LEU |
| 43 | oo | 85 | LEU |
| 43 | oo | 93 | LEU |
| 44 | pp | 10 | ILE |
| 44 | pp | 11 | THR |
| 44 | pp | 20 | SER |
| 44 | pp | 40 | SER |
| 44 | pp | 46 | CYS |
| 44 | pp | 49 | ARG |
| 44 | pp | 58 | SER |
| 44 | pp | 60 | CYS |
| 44 | pp | 71 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | pp | 81 | SER |
| 44 | pp | 84 | ARG |
| 45 | qq | 3 | LYS |
| 45 | qq | 8 | HIS |
| 45 | qq | 34 | LEU |
| 45 | qq | 49 | PHE |
| 45 | qq | 67 | ILE |
| 45 | qq | 97 | LYS |
| 45 | qq | 102 | LYS |
| 45 | qq | 105 | LYS |
| 45 | qq | 107 | TYR |
| 45 | qq | 122 | ARG |
| 45 | qq | 177 | ASP |
| 45 | qq | 179 | LEU |
| 45 | qq | 191 | VAL |
| 45 | qq | 198 | TRP |
| 45 | qq | 199 | GLN |
| 45 | qq | 207 | LYS |
| 45 | qq | 214 | TYR |
| 46 | rr | 20 | TYR |
| 46 | rr | 35 | VAL |
| 46 | rr | 37 | SER |
| 46 | rr | 39 | GLN |
| 46 | rr | 48 | ARG |
| 46 | rr | 62 | ARG |
| 46 | rr | 90 | PHE |
| 46 | rr | 91 | THR |
| 46 | rr | 120 | ASP |
| 46 | rr | 122 | TRP |
| 46 | rr | 134 | LYS |
| 46 | rr | 135 | THR |
| 46 | rr | 149 | ARG |
| 46 | rr | 187 | LEU |
| 46 | rr | 195 | ASN |
| 48 | A | 9 | LEU |
| 48 | A | 34 | GLU |
| 48 | A | 56 | LYS |
| 48 | A | 79 | ARG |
| 48 | A | 109 | ASN |
| 48 | A | 134 | LYS |
| 48 | A | 135 | GLU |
| 48 | A | 146 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | A | 150 | ASP |
| 48 | A | 173 | ILE |
| 48 | A | 177 | LEU |
| 48 | A | 195 | TRP |
| 48 | A | 197 | ILE |
| 48 | A | 198 | MET |
| 48 | A | 205 | ARG |
| 49 | B | 47 | LEU |
| 49 | B | 48 | VAL |
| 49 | B | 70 | LEU |
| 49 | B | 81 | PHE |
| 49 | B | 84 | VAL |
| 49 | B | 89 | ASP |
| 49 | B | 96 | LEU |
| 49 | B | 99 | ASN |
| 49 | B | 100 | PHE |
| 49 | B | 118 | GLN |
| 49 | B | 119 | THR |
| 49 | B | 120 | LEU |
| 49 | B | 127 | VAL |
| 49 | B | 145 | LYS |
| 49 | B | 179 | SER |
| 49 | B | 181 | LEU |
| 49 | B | 191 | GLU |
| 49 | B | 208 | GLN |
| 50 | C | 49 | LEU |
| 50 | C | 51 | LYS |
| 50 | C | 71 | PHE |
| 50 | C | 82 | LYS |
| 50 | C | 86 | MET |
| 50 | C | 88 | ILE |
| 50 | C | 89 | LYS |
| 50 | C | 94 | GLN |
| 50 | C | 99 | GLN |
| 50 | C | 100 | ARG |
| 50 | C | 111 | ASP |
| 50 | C | 122 | THR |
| 50 | C | 142 | ILE |
| 50 | C | 145 | ARG |
| 50 | C | 146 | ARG |
| 50 | C | 149 | TRP |
| 50 | C | 166 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | C | 169 | SER |
| 50 | C | 174 | LEU |
| 50 | C | 186 | SER |
| 50 | C | 212 | LEU |
| 50 | C | 225 | ASN |
| 50 | C | 234 | LEU |
| 50 | C | 235 | TRP |
| 51 | D | 5 | ILE |
| 51 | D | 7 | LYS |
| 51 | D | 11 | LEU |
| 51 | D | 51 | ARG |
| 51 | D | 65 | ARG |
| 51 | D | 113 | LEU |
| 51 | D | 122 | VAL |
| 51 | D | 134 | CYS |
| 51 | D | 135 | GLU |
| 51 | D | 139 | SER |
| 51 | D | 141 | LYS |
| 51 | D | 143 | ARG |
| 51 | D | 157 | LEU |
| 51 | D | 158 | ILE |
| 51 | D | 162 | GLN |
| 51 | D | 173 | ARG |
| 51 | D | 177 | LEU |
| 51 | D | 178 | ARG |
| 51 | D | 179 | GLN |
| 51 | D | 222 | VAL |
| 52 | E | 6 | LYS |
| 52 | E | 9 | LEU |
| 52 | E | 18 | TRP |
| 52 | E | 37 | LYS |
| 52 | E | 38 | LEU |
| 52 | E | 42 | LEU |
| 52 | E | 51 | ARG |
| 52 | E | 68 | ARG |
| 52 | E | 77 | ARG |
| 52 | E | 79 | ASP |
| 52 | E | 123 | LEU |
| 52 | E | 127 | LYS |
| 52 | E | 133 | LYS |
| 52 | E | 139 | VAL |
| 52 | E | 143 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | E | 159 | THR |
| 52 | E | 163 | ASP |
| 52 | E | 176 | ASP |
| 52 | E | 187 | ARG |
| 52 | E | 206 | ASP |
| 52 | E | 208 | VAL |
| 52 | E | 225 | VAL |
| 52 | E | 245 | LYS |
| 52 | E | 247 | THR |
| 53 | F | 101 | MET |
| 53 | F | 114 | ARG |
| 53 | F | 121 | GLU |
| 53 | F | 158 | ARG |
| 53 | F | 186 | PHE |
| 53 | F | 188 | ASN |
| 53 | F | 192 | ILE |
| 53 | F | 196 | LEU |
| 53 | F | 220 | GLU |
| 54 | G | 52 | ILE |
| 54 | G | 75 | LEU |
| 54 | G | 81 | HIS |
| 54 | G | 92 | ARG |
| 54 | G | 95 | LYS |
| 54 | G | 96 | SER |
| 54 | G | 141 | ILE |
| 54 | G | 152 | ASP |
| 54 | G | 159 | ARG |
| 54 | G | 164 | LYS |
| 54 | G | 178 | LEU |
| 54 | G | 182 | GLN |
| 54 | G | 215 | ARG |
| 55 | H | 11 | GLN |
| 55 | H | 16 | LEU |
| 55 | H | 47 | ARG |
| 55 | H | 80 | GLU |
| 55 | H | 81 | LEU |
| 55 | H | 110 | GLN |
| 55 | H | 114 | ARG |
| 55 | H | 126 | LEU |
| 55 | H | 139 | ARG |
| 55 | H | 168 | SER |
| 55 | H | 174 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55 | H | 180 | GLN |
| 56 | I | 8 | ARG |
| 56 | I | 10 | LYS |
| 56 | I | 24 | LYS |
| 56 | I | 25 | ARG |
| 56 | I | 29 | LEU |
| 56 | I | 62 | THR |
| 56 | I | 72 | VAL |
| 56 | I | 75 | LYS |
| 56 | I | 77 | ARG |
| 56 | I | 86 | SER |
| 56 | I | 92 | ARG |
| 56 | I | 101 | ILE |
| 56 | I | 138 | LYS |
| 56 | I | 140 | THR |
| 56 | I | 144 | TRP |
| 56 | I | 161 | PHE |
| 56 | I | 170 | ILE |
| 57 | J | 28 | LEU |
| 57 | J | 30 | LEU |
| 57 | J | 37 | LYS |
| 57 | J | 49 | LEU |
| 57 | J | 69 | ARG |
| 57 | J | 83 | ILE |
| 57 | J | 86 | LEU |
| 57 | J | 89 | ASP |
| 57 | J | 93 | LEU |
| 57 | J | 94 | ASP |
| 57 | J | 126 | ARG |
| 57 | J | 132 | ARG |
| 57 | J | 145 | SER |
| 57 | J | 149 | ARG |
| 57 | J | 175 | LYS |
| 57 | J | 176 | ARG |
| 58 | K | 20 | VAL |
| 58 | K | 40 | LEU |
| 58 | K | 54 | PHE |
| 58 | K | 55 | VAL |
| 58 | K | 59 | PHE |
| 58 | K | 76 | LEU |
| 58 | K | 86 | ILE |
| 59 | L | 8 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | L | 55 | ASP |
| 59 | L | 67 | ARG |
| 59 | L | 77 | SER |
| 59 | L | 80 | MET |
| 59 | L | 83 | THR |
| 59 | L | 84 | ILE |
| 59 | L | 87 | ARG |
| 59 | L | 90 | TYR |
| 59 | L | 105 | LYS |
| 59 | L | 125 | VAL |
| 59 | L | 136 | ARG |
| 59 | L | 153 | PHE |
| 60 | M | 55 | LEU |
| 60 | M | 67 | LEU |
| 60 | M | 91 | TRP |
| 60 | M | 104 | ARG |
| 60 | M | 105 | LYS |
| 61 | N | 3 | ARG |
| 61 | N | 12 | SER |
| 61 | N | 17 | PRO |
| 61 | N | 25 | TRP |
| 61 | N | 49 | GLN |
| 61 | N | 64 | LYS |
| 61 | N | 72 | LEU |
| 61 | N | 88 | LEU |
| 61 | N | 89 | TYR |
| 61 | N | 115 | LEU |
| 61 | N | 119 | GLU |
| 61 | N | 121 | ARG |
| 61 | N | 124 | ARG |
| 61 | N | 139 | TRP |
| 61 | N | 142 | GLU |
| 62 | O | 37 | GLU |
| 62 | O | 51 | ASP |
| 62 | O | 58 | TYR |
| 62 | O | 67 | VAL |
| 62 | O | 71 | CYS |
| 62 | O | 86 | THR |
| 62 | O | 110 | LEU |
| 62 | O | 114 | ARG |
| 62 | O | 124 | ASP |
| 63 | P | 17 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63 | P | 18 | LYS |
| 63 | P | 21 | ASP |
| 63 | P | 32 | ASP |
| 63 | P | 40 | ARG |
| 63 | P | 43 | ARG |
| 63 | P | 52 | LYS |
| 63 | P | 57 | MET |
| 63 | P | 79 | HIS |
| 63 | P | 81 | ARG |
| 63 | P | 84 | ILE |
| 63 | P | 89 | MET |
| 63 | P | 127 | ARG |
| 64 | Q | 19 | VAL |
| 64 | Q | 53 | LEU |
| 64 | Q | 121 | SER |
| 64 | Q | 125 | GLU |
| 64 | Q | 128 | LYS |
| 64 | Q | 142 | TYR |
| 65 | R | 5 | ARG |
| 65 | R | 6 | THR |
| 65 | R | 16 | LEU |
| 65 | R | 47 | ARG |
| 65 | R | 56 | HIS |
| 65 | R | 66 | VAL |
| 65 | R | 88 | VAL |
| 65 | R | 127 | VAL |
| 65 | R | 128 | ARG |
| 65 | R | 130 | ARG |
| 66 | S | 16 | ARG |
| 66 | S | 36 | ARG |
| 66 | S | 41 | ARG |
| 66 | S | 49 | LYS |
| 66 | S | 73 | MET |
| 66 | S | 74 | GLN |
| 66 | S | 84 | TRP |
| 66 | S | 93 | ASN |
| 66 | S | 96 | LYS |
| 66 | S | 100 | SER |
| 66 | S | 105 | LEU |
| 66 | S | 126 | ARG |
| 66 | S | 131 | LEU |
| 66 | S | 136 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66 | S | 137 | HIS |
| 66 | S | 144 | ARG |
| 67 | T | 7 | ARG |
| 67 | T | 57 | ARG |
| 67 | T | 60 | SER |
| 67 | T | 63 | ARG |
| 67 | T | 68 | ARG |
| 67 | T | 85 | ASN |
| 67 | T | 86 | ARG |
| 68 | U | 52 | LYS |
| 68 | U | 85 | ARG |
| 68 | U | 86 | ILE |
| 68 | U | 94 | GLU |
| 69 | V | 12 | TYR |
| 69 | V | 17 | CYS |
| 69 | V | 28 | ASP |
| 69 | V | 33 | GLN |
| 69 | V | 38 | GLN |
| 69 | V | 56 | SER |
| 69 | V | 60 | ARG |
| 69 | V | 67 | ASP |
| 70 | W | 2 | THR |
| 70 | W | 15 | ASN |
| 70 | W | 23 | ARG |
| 70 | W | 24 | GLN |
| 70 | W | 25 | VAL |
| 70 | W | 26 | LEU |
| 70 | W | 28 | ARG |
| 70 | W | 40 | VAL |
| 70 | W | 51 | GLU |
| 70 | W | 61 | ILE |
| 70 | W | 66 | ASN |
| 70 | W | 70 | ASN |
| 70 | W | 83 | ILE |
| 70 | W | 107 | SER |
| 70 | W | 111 | MET |
| 70 | W | 130 | TYR |
| 71 | X | 9 | LEU |
| 71 | X | 19 | ARG |
| 71 | X | 23 | ARG |
| 71 | X | 63 | GLN |
| 71 | X | 70 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71 | X | 71 | CYS |
| 71 | X | 84 | THR |
| 71 | X | 98 | GLU |
| 71 | X | 99 | ASN |
| 71 | X | 102 | VAL |
| 71 | X | 107 | PHE |
| 71 | X | 109 | ARG |
| 71 | X | 130 | VAL |
| 72 | Y | 3 | ASP |
| 72 | Y | 6 | THR |
| 72 | Y | 27 | VAL |
| 72 | Y | 31 | ASN |
| 72 | Y | 46 | GLU |
| 72 | Y | 98 | GLU |
| 72 | Y | 110 | GLN |
| 72 | Y | 116 | LYS |
| 72 | Y | 121 | THR |
| 73 | Z | 68 | ARG |
| 73 | Z | 77 | ARG |
| 73 | Z | 97 | LYS |
| 74 | a | 5 | ARG |
| 74 | a | 7 | SER |
| 74 | a | 8 | ASN |
| 74 | a | 18 | VAL |
| 74 | a | 23 | CYS |
| 74 | a | 28 | ARG |
| 74 | a | 32 | LYS |
| 74 | a | 39 | MET |
| 74 | a | 50 | ILE |
| 74 | a | 64 | LEU |
| 74 | a | 75 | ILE |
| 74 | a | 76 | SER |
| 75 | b | 7 | LEU |
| 75 | b | 9 | HIS |
| 75 | b | 21 | LEU |
| 75 | b | 67 | THR |
| 76 | c | 16 | LEU |
| 76 | c | 32 | PHE |
| 76 | c | 56 | LEU |
| 77 | d | 21 | CYS |
| 77 | d | 40 | ARG |
| 77 | d | 49 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78 | e | 17 | GLN |
| 78 | e | 22 | GLU |
| 78 | e | 33 | ARG |
| 79 | f | 89 | LYS |
| 79 | f | 97 | LYS |
| 79 | f | 100 | LEU |
| 79 | f | 106 | TYR |
| 79 | f | 113 | LYS |
| 79 | f | 114 | VAL |
| 79 | f | 117 | LEU |
| 79 | f | 120 | GLU |
| 79 | f | 136 | ARG |
| 79 | f | 139 | CYS |
| 80 | g | 27 | SER |
| 80 | g | 43 | LEU |
| 80 | g | 52 | GLU |
| 80 | g | 55 | PHE |
| 80 | g | 60 | ARG |
| 80 | g | 67 | HIS |
| 80 | g | 75 | SER |
| 80 | g | 99 | ASN |
| 80 | g | 175 | VAL |
| 80 | g | 188 | LEU |
| 80 | g | 238 | PHE |
| 80 | g | 242 | ASP |
| 80 | g | 244 | LYS |
| 80 | g | 270 | TYR |
| 80 | g | 273 | GLU |
| 80 | g | 275 | GLU |
| 80 | g | 292 | GLN |
| 80 | g | 299 | LEU |
| 80 | g | 321 | GLN |
| 83 | 1 | 13 | MET |
| 83 | 1 | 21 | ASN |
| 83 | 1 | 23 | SER |
| 83 | 1 | 24 | VAL |
| 83 | 1 | 25 | ILE |
| 83 | 1 | 29 | ASP |
| 83 | 1 | 35 | LEU |
| 83 | 1 | 42 | ARG |
| 83 | 1 | 45 | ILE |
| 83 | 1 | 57 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 83 | 1 | 61 | LYS |
| 83 | 1 | 64 | GLN |
| 83 | 1 | 78 | TYR |
| 83 | 1 | 79 | SER |
| 83 | 1 | 80 | GLU |
| 83 | 1 | 126 | LEU |
| 83 | 1 | 128 | VAL |
| 83 | 1 | 136 | CYS |
| 83 | 1 | 142 | VAL |
| 83 | 1 | 150 | ARG |
| 83 | 1 | 161 | ASP |
| 83 | 1 | 164 | LEU |
| 83 | 1 | 166 | GLU |
| 83 | 1 | 171 | LYS |
| 83 | 1 | 173 | ASP |
| 83 | 1 | 202 | VAL |
| 83 | 1 | 208 | THR |
| 83 | 1 | 229 | TYR |
| 83 | 1 | 236 | ASP |
| 83 | 1 | 237 | LYS |
| 83 | 1 | 248 | SER |
| 83 | 1 | 251 | ASN |
| 83 | 1 | 276 | PHE |
| 83 | 1 | 289 | MET |
| 83 | 1 | 293 | LYS |
| 83 | 1 | 305 | ILE |
| 83 | 1 | 313 | ASP |
| 83 | 1 | 315 | GLU |
| 83 | 1 | 324 | MET |
| 83 | 1 | 344 | SER |
| 83 | 1 | 379 | MET |
| 83 | 1 | 380 | LEU |
| 83 | 1 | 381 | TYR |
| 83 | 1 | 383 | SER |
| 83 | 1 | 385 | MET |
| 83 | 1 | 391 | LYS |
| 83 | 1 | 394 | PHE |
| 83 | 1 | 433 | ARG |
| 83 | 1 | 441 | PHE |
| 83 | 1 | 463 | LEU |
| 83 | 1 | 477 | ASN |
| 83 | 1 | 481 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 83 | 1 | 482 | LYS |
| 83 | 1 | 495 | VAL |
| 83 | 1 | 508 | LEU |
| 83 | 1 | 510 | ARG |
| 83 | 1 | 515 | ASP |
| 83 | 1 | 519 | LEU |
| 83 | 1 | 521 | TYR |
| 83 | 1 | 535 | GLU |
| 83 | 1 | 555 | LYS |
| 83 | 1 | 557 | SER |
| 83 | 1 | 561 | VAL |
| 83 | 1 | 570 | GLU |
| 83 | 1 | 574 | THR |
| 83 | 1 | 582 | LYS |
| 83 | 1 | 586 | ILE |
| 83 | 1 | 622 | ASP |
| 83 | 1 | 646 | VAL |
| 83 | 1 | 651 | LYS |
| 83 | 1 | 653 | VAL |
| 83 | 1 | 669 | TRP |
| 83 | 1 | 671 | THR |
| 83 | 1 | 680 | GLU |
| 83 | 1 | 681 | MET |
| 83 | 1 | 682 | ARG |
| 83 | 1 | 689 | LEU |
| 83 | 1 | 693 | LEU |
| 83 | 1 | 694 | HIS |
| 83 | 1 | 696 | ASP |
| 83 | 1 | 698 | ILE |
| 83 | 1 | 708 | THR |
| 83 | 1 | 721 | ASP |
| 83 | 1 | 727 | PRO |
| 83 | 1 | 738 | GLN |
| 83 | 1 | 775 | ASN |
| 83 | 1 | 785 | ARG |
| 83 | 1 | 803 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AA | 97 | ASN |
| 4 | AA | 132 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 4 | AA | 187 | HIS |
| 4 | AA | 209 | HIS |
| 4 | AA | 211 | HIS |
| 4 | AA | 233 | GLN |
| 5 | BB | 173 | GLN |
| 5 | BB | 177 | HIS |
| 5 | BB | 274 | HIS |
| 5 | BB | 313 | HIS |
| 5 | BB | 371 | GLN |
| 6 | CC | 36 | HIS |
| 6 | CC | 48 | GLN |
| 6 | CC | 157 | GLN |
| 6 | CC | 307 | GLN |
| 7 | DD | 13 | HIS |
| 7 | DD | 39 | GLN |
| 8 | EE | 171 | HIS |
| 9 | FF | 90 | ASN |
| 9 | FF | 241 | ASN |
| 10 | GG | 137 | HIS |
| 10 | GG | 144 | ASN |
| 10 | GG | 220 | ASN |
| 11 | HH | 5 | GLN |
| 11 | HH | 50 | ASN |
| 12 | II | 14 | ASN |
| 12 | II | 144 | ASN |
| 14 | LL | 114 | GLN |
| 17 | OO | 91[A] | HIS |
| 18 | PP | 42 | GLN |
| 19 | QQ | 73 | GLN |
| 19 | QQ | 166 | GLN |
| 20 | RR | 130 | ASN |
| 21 | SS | 88 | HIS |
| 22 | TT | 49 | HIS |
| 22 | TT | 54 | HIS |
| 22 | TT | 146 | ASN |
| 24 | VV | 98 | ASN |
| 24 | VV | 132 | ASN |
| 26 | XX | 137 | ASN |
| 28 | ZZ | 79 | HIS |
| 29 | aa | 41 | HIS |
| 29 | aa | 44 | ASN |
| 30 | bb | 12 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | dd | 57 | GLN |
| 33 | ee | 35 | GLN |
| 35 | gg | 52 | GLN |
| 37 | ii | 19 | GLN |
| 38 | jj | 47 | HIS |
| 38 | jj | 69 | HIS |
| 39 | kk | 32 | ASN |
| 45 | qq | 12 | HIS |
| 45 | qq | 94 | ASN |
| 45 | qq | 199 | GLN |
| 46 | rr | 39 | GLN |
| 46 | rr | 191 | GLN |
| 46 | rr | 195 | ASN |
| 48 | A | 109 | ASN |
| 49 | B | 178 | ASN |
| 50 | C | 115 | HIS |
| 50 | C | 152 | ASN |
| 51 | D | 179 | GLN |
| 52 | E | 67 | GLN |
| 53 | F | 81 | ASN |
| 53 | F | 172 | GLN |
| 53 | F | 202 | ASN |
| 54 | G | 176 | GLN |
| 54 | G | 190 | GLN |
| 57 | J | 48 | GLN |
| 59 | L | 14 | GLN |
| 59 | L | 37 | ASN |
| 61 | N | 49 | GLN |
| 62 | O | 29 | HIS |
| 63 | P | 79 | HIS |
| 64 | Q | 83 | GLN |
| 66 | S | 89 | GLN |
| 66 | S | 137 | HIS |
| 67 | T | 25 | GLN |
| 67 | T | 85 | ASN |
| 69 | V | 33 | GLN |
| 70 | W | 64 | GLN |
| 71 | X | 18 | HIS |
| 71 | X | 22 | ASN |
| 71 | X | 79 | ASN |
| 71 | X | 99 | ASN |
| 72 | Y | 29 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72 | Y | 31 | ASN |
| 73 | Z | 95 | HIS |
| 75 | b | 49 | HIS |
| 80 | g | 321 | GLN |
| 83 | 1 | 30 | HIS |
| 83 | 1 | 101 | ASN |
| 83 | 1 | 432 | GLN |
| 83 | 1 | 583 | HIS |
| 83 | 1 | 584 | ASN |
| 83 | 1 | 644 | ASN |
| 83 | 1 | 699 | HIS |
| 83 | 1 | 704 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 5 | 3265/3270 (99%) | 984 (30%) | 198 (6%) |
| 2 | 7 | 120/121 (99%) | 22 (18%) | 4 (3%) |
| 3 | 8 | 156/157 (99%) | 40 (25%) | 6 (3%) |
| 81 | 2 | 1778/1798 (98%) | 790 (44%) | 127 (7%) |
| 82 | 4 | 184/190 (96%) | 90 (48%) | 24 (13%) |
| All | All | 5503/5536 (99%) | 1926 (34%) | 359 (6%) |

All (1926) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 6 | A |
| 1 | 5 | 15 | C |
| 1 | 5 | 18 | G |
| 1 | 5 | 21 | G |
| 1 | 5 | 22 | G |
| 1 | 5 | 26 | A |
| 1 | 5 | 40 | A |
| 1 | 5 | 43 | A |
| 1 | 5 | 44 | U |
| 1 | 5 | 45 | A |
| 1 | 5 | 48 | A |
| 1 | 5 | 49 | A |
| 1 | 5 | 57 | A |
| 1 | 5 | 59 | G |
| 1 | 5 | 60 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 65 | A |
| 1 | 5 | 66 | A |
| 1 | 5 | 68 | C |
| 1 | 5 | 73 | C |
| 1 | 5 | 75 | G |
| 1 | 5 | 76 | G |
| 1 | 5 | 85 | A |
| 1 | 5 | 87 | U |
| 1 | 5 | 92 | G |
| 1 | 5 | 96 | G |
| 1 | 5 | 99 | A |
| 1 | 5 | 109 | A |
| 1 | 5 | 110 | G |
| 1 | 5 | 111 | C |
| 1 | 5 | 113 | C |
| 1 | 5 | 115 | A |
| 1 | 5 | 117 | U |
| 1 | 5 | 120 | G |
| 1 | 5 | 121 | A |
| 1 | 5 | 122 | A |
| 1 | 5 | 128 | G |
| 1 | 5 | 133 | U |
| 1 | 5 | 134 | U |
| 1 | 5 | 136 | G |
| 1 | 5 | 143 | G |
| 1 | 5 | 146 | U |
| 1 | 5 | 150 | A |
| 1 | 5 | 156 | A |
| 1 | 5 | 157 | A |
| 1 | 5 | 161 | G |
| 1 | 5 | 165 | A |
| 1 | 5 | 166 | C |
| 1 | 5 | 167 | U |
| 1 | 5 | 168 | U |
| 1 | 5 | 169 | U |
| 1 | 5 | 170 | G |
| 1 | 5 | 171 | U |
| 1 | 5 | 174 | C |
| 1 | 5 | 177 | G |
| 1 | 5 | 182 | U |
| 1 | 5 | 187 | A |
| 1 | 5 | 190 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 191 | U |
| 1 | 5 | 198 | A |
| 1 | 5 | 200 | C |
| 1 | 5 | 210 | U |
| 1 | 5 | 211 | A |
| 1 | 5 | 213 | A |
| 1 | 5 | 218 | G |
| 1 | 5 | 219 | A |
| 1 | 5 | 220 | G |
| 1 | 5 | 221 | A |
| 1 | 5 | 224 | C |
| 1 | 5 | 234 | G |
| 1 | 5 | 239 | U |
| 1 | 5 | 240 | C |
| 1 | 5 | 241 | C |
| 1 | 5 | 244 | G |
| 1 | 5 | 248 | U |
| 1 | 5 | 249 | U |
| 1 | 5 | 250 | U |
| 1 | 5 | 251 | G |
| 1 | 5 | 252 | U |
| 1 | 5 | 253 | A |
| 1 | 5 | 254 | A |
| 1 | 5 | 266 | C |
| 1 | 5 | 269 | G |
| 1 | 5 | 282 | G |
| 1 | 5 | 283 | G |
| 1 | 5 | 284 | A |
| 1 | 5 | 285 | A |
| 1 | 5 | 286 | U |
| 1 | 5 | 295 | A |
| 1 | 5 | 298 | U |
| 1 | 5 | 299 | G |
| 1 | 5 | 305 | U |
| 1 | 5 | 306 | A |
| 1 | 5 | 307 | A |
| 1 | 5 | 315 | C |
| 1 | 5 | 319 | A |
| 1 | 5 | 323 | A |
| 1 | 5 | 329 | U |
| 1 | 5 | 336 | A |
| 1 | 5 | 338 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 339 | C |
| 1 | 5 | 343 | U |
| 1 | 5 | 349 | A |
| 1 | 5 | 350 | C |
| 1 | 5 | 368 | G |
| 1 | 5 | 370 | U |
| 1 | 5 | 374 | A |
| 1 | 5 | 376 | G |
| 1 | 5 | 378 | A |
| 1 | 5 | 385 | A |
| 1 | 5 | 395 | A |
| 1 | 5 | 398 | A |
| 1 | 5 | 399 | A |
| 1 | 5 | 401 | U |
| 1 | 5 | 403 | C |
| 1 | 5 | 404 | G |
| 1 | 5 | 407 | A |
| 1 | 5 | 420 | G |
| 1 | 5 | 421 | G |
| 1 | 5 | 422 | A |
| 1 | 5 | 429 | U |
| 1 | 5 | 436 | A |
| 1 | 5 | 437 | G |
| 1 | 5 | 438 | A |
| 1 | 5 | 439 | C |
| 1 | 5 | 440 | A |
| 1 | 5 | 441 | U |
| 1 | 5 | 443 | G |
| 1 | 5 | 478 | U |
| 1 | 5 | 486 | U |
| 1 | 5 | 487 | U |
| 1 | 5 | 491 | U |
| 1 | 5 | 492 | A |
| 1 | 5 | 494 | A |
| 1 | 5 | 503 | A |
| 1 | 5 | 506 | G |
| 1 | 5 | 507 | U |
| 1 | 5 | 512 | C |
| 1 | 5 | 514 | G |
| 1 | 5 | 518 | C |
| 1 | 5 | 519 | G |
| 1 | 5 | 520 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 521 | U |
| 1 | 5 | 525 | G |
| 1 | 5 | 528 | U |
| 1 | 5 | 529 | U |
| 1 | 5 | 530 | A |
| 1 | 5 | 531 | U |
| 1 | 5 | 532 | A |
| 1 | 5 | 533 | G |
| 1 | 5 | 537 | G |
| 1 | 5 | 542 | A |
| 1 | 5 | 543 | A |
| 1 | 5 | 545 | A |
| 1 | 5 | 551 | A |
| 1 | 5 | 552 | G |
| 1 | 5 | 565 | A |
| 1 | 5 | 567 | U |
| 1 | 5 | 573 | U |
| 1 | 5 | 575 | U |
| 1 | 5 | 577 | G |
| 1 | 5 | 580 | A |
| 1 | 5 | 581 | A |
| 1 | 5 | 582 | G |
| 1 | 5 | 584 | A |
| 1 | 5 | 589 | G |
| 1 | 5 | 590 | G |
| 1 | 5 | 594 | A |
| 1 | 5 | 595 | A |
| 1 | 5 | 596 | U |
| 1 | 5 | 597 | G |
| 1 | 5 | 598 | G |
| 1 | 5 | 609 | C |
| 1 | 5 | 615 | U |
| 1 | 5 | 620 | A |
| 1 | 5 | 622 | A |
| 1 | 5 | 633 | A |
| 1 | 5 | 640 | C |
| 1 | 5 | 644 | U |
| 1 | 5 | 650 | A |
| 1 | 5 | 654 | U |
| 1 | 5 | 660 | U |
| 1 | 5 | 664 | A |
| 1 | 5 | 670 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 671 | U |
| 1 | 5 | 672 | A |
| 1 | 5 | 678 | A |
| 1 | 5 | 681 | G |
| 1 | 5 | 683 | A |
| 1 | 5 | 685 | G |
| 1 | 5 | 688 | A |
| 1 | 5 | 694 | G |
| 1 | 5 | 698 | A |
| 1 | 5 | 699 | G |
| 1 | 5 | 708 | A |
| 1 | 5 | 709 | G |
| 1 | 5 | 721 | G |
| 1 | 5 | 724 | C |
| 1 | 5 | 729 | C |
| 1 | 5 | 736 | C |
| 1 | 5 | 737 | U |
| 1 | 5 | 738 | U |
| 1 | 5 | 741 | G |
| 1 | 5 | 742 | A |
| 1 | 5 | 745 | G |
| 1 | 5 | 747 | U |
| 1 | 5 | 748 | U |
| 1 | 5 | 751 | A |
| 1 | 5 | 752 | G |
| 1 | 5 | 755 | A |
| 1 | 5 | 756 | G |
| 1 | 5 | 757 | A |
| 1 | 5 | 758 | G |
| 1 | 5 | 770 | G |
| 1 | 5 | 772 | A |
| 1 | 5 | 777 | A |
| 1 | 5 | 778 | A |
| 1 | 5 | 779 | A |
| 1 | 5 | 788 | A |
| 1 | 5 | 794 | C |
| 1 | 5 | 797 | G |
| 1 | 5 | 801 | A |
| 1 | 5 | 805 | U |
| 1 | 5 | 808 | A |
| 1 | 5 | 817 | A |
| 1 | 5 | 832 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 842 | U |
| 1 | 5 | 845 | U |
| 1 | 5 | 850 | U |
| 1 | 5 | 861 | C |
| 1 | 5 | 867 | A |
| 1 | 5 | 868 | U |
| 1 | 5 | 878 | G |
| 1 | 5 | 879 | G |
| 1 | 5 | 885 | A |
| 1 | 5 | 886 | A |
| 1 | 5 | 887 | G |
| 1 | 5 | 888 | A |
| 1 | 5 | 890 | U |
| 1 | 5 | 891 | A |
| 1 | 5 | 892 | A |
| 1 | 5 | 894 | C |
| 1 | 5 | 908 | G |
| 1 | 5 | 915 | C |
| 1 | 5 | 924 | G |
| 1 | 5 | 930 | C |
| 1 | 5 | 931 | U |
| 1 | 5 | 932 | C |
| 1 | 5 | 933 | A |
| 1 | 5 | 941 | A |
| 1 | 5 | 945 | G |
| 1 | 5 | 949 | G |
| 1 | 5 | 950 | U |
| 1 | 5 | 951 | A |
| 1 | 5 | 952 | U |
| 1 | 5 | 953 | C |
| 1 | 5 | 955 | G |
| 1 | 5 | 962 | G |
| 1 | 5 | 965 | G |
| 1 | 5 | 972 | G |
| 1 | 5 | 973 | A |
| 1 | 5 | 974 | A |
| 1 | 5 | 981 | G |
| 1 | 5 | 986 | A |
| 1 | 5 | 987 | C |
| 1 | 5 | 988 | C |
| 1 | 5 | 989 | G |
| 1 | 5 | 990 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 992 | G |
| 1 | 5 | 994 | U |
| 1 | 5 | 995 | G |
| 1 | 5 | 996 | A |
| 1 | 5 | 997 | A |
| 1 | 5 | 999 | U |
| 1 | 5 | 1000 | G |
| 1 | 5 | 1003 | C |
| 1 | 5 | 1005 | U |
| 1 | 5 | 1006 | G |
| 1 | 5 | 1018 | A |
| 1 | 5 | 1020 | C |
| 1 | 5 | 1025 | A |
| 1 | 5 | 1034 | G |
| 1 | 5 | 1035 | A |
| 1 | 5 | 1036 | A |
| 1 | 5 | 1043 | G |
| 1 | 5 | 1052 | U |
| 1 | 5 | 1053 | U |
| 1 | 5 | 1056 | A |
| 1 | 5 | 1058 | G |
| 1 | 5 | 1064 | A |
| 1 | 5 | 1065 | U |
| 1 | 5 | 1066 | U |
| 1 | 5 | 1067 | U |
| 1 | 5 | 1069 | A |
| 1 | 5 | 1074 | A |
| 1 | 5 | 1075 | G |
| 1 | 5 | 1078 | C |
| 1 | 5 | 1087 | G |
| 1 | 5 | 1088 | G |
| 1 | 5 | 1102 | G |
| 1 | 5 | 1115 | U |
| 1 | 5 | 1116 | G |
| 1 | 5 | 1122 | U |
| 1 | 5 | 1123 | G |
| 1 | 5 | 1124 | A |
| 1 | 5 | 1129 | A |
| 1 | 5 | 1130 | A |
| 1 | 5 | 1145 | G |
| 1 | 5 | 1146 | C |
| 1 | 5 | 1149 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1151 | A |
| 1 | 5 | 1152 | U |
| 1 | 5 | 1153 | A |
| 1 | 5 | 1156 | C |
| 1 | 5 | 1162 | U |
| 1 | 5 | 1163 | C |
| 1 | 5 | 1164 | A |
| 1 | 5 | 1167 | C |
| 1 | 5 | 1168 | A |
| 1 | 5 | 1172 | C |
| 1 | 5 | 1177 | G |
| 1 | 5 | 1179 | U |
| 1 | 5 | 1180 | G |
| 1 | 5 | 1191 | U |
| 1 | 5 | 1192 | A |
| 1 | 5 | 1193 | G |
| 1 | 5 | 1194 | A |
| 1 | 5 | 1195 | C |
| 1 | 5 | 1196 | A |
| 1 | 5 | 1197 | G |
| 1 | 5 | 1198 | C |
| 1 | 5 | 1203 | C |
| 1 | 5 | 1206 | U |
| 1 | 5 | 1207 | G |
| 1 | 5 | 1208 | G |
| 1 | 5 | 1210 | C |
| 1 | 5 | 1212 | U |
| 1 | 5 | 1213 | G |
| 1 | 5 | 1216 | A |
| 1 | 5 | 1217 | G |
| 1 | 5 | 1218 | U |
| 1 | 5 | 1223 | A |
| 1 | 5 | 1225 | C |
| 1 | 5 | 1229 | U |
| 1 | 5 | 1230 | A |
| 1 | 5 | 1234 | A |
| 1 | 5 | 1235 | G |
| 1 | 5 | 1236 | U |
| 1 | 5 | 1237 | G |
| 1 | 5 | 1248 | C |
| 1 | 5 | 1254 | C |
| 1 | 5 | 1256 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1257 | A |
| 1 | 5 | 1258 | A |
| 1 | 5 | 1263 | C |
| 1 | 5 | 1266 | G |
| 1 | 5 | 1272 | A |
| 1 | 5 | 1274 | A |
| 1 | 5 | 1276 | U |
| 1 | 5 | 1278 | G |
| 1 | 5 | 1279 | A |
| 1 | 5 | 1280 | U |
| 1 | 5 | 1281 | G |
| 1 | 5 | 1284 | G |
| 1 | 5 | 1289 | A |
| 1 | 5 | 1296 | U |
| 1 | 5 | 1301 | A |
| 1 | 5 | 1302 | U |
| 1 | 5 | 1319 | U |
| 1 | 5 | 1320 | A |
| 1 | 5 | 1321 | A |
| 1 | 5 | 1322 | U |
| 1 | 5 | 1323 | A |
| 1 | 5 | 1324 | U |
| 1 | 5 | 1326 | A |
| 1 | 5 | 1327 | U |
| 1 | 5 | 1328 | G |
| 1 | 5 | 1351 | G |
| 1 | 5 | 1356 | C |
| 1 | 5 | 1357 | A |
| 1 | 5 | 1370 | A |
| 1 | 5 | 1371 | G |
| 1 | 5 | 1390 | A |
| 1 | 5 | 1398 | U |
| 1 | 5 | 1401 | U |
| 1 | 5 | 1402 | G |
| 1 | 5 | 1405 | G |
| 1 | 5 | 1408 | C |
| 1 | 5 | 1409 | U |
| 1 | 5 | 1414 | G |
| 1 | 5 | 1417 | A |
| 1 | 5 | 1421 | G |
| 1 | 5 | 1422 | C |
| 1 | 5 | 1424 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1425 | A |
| 1 | 5 | 1426 | U |
| 1 | 5 | 1427 | A |
| 1 | 5 | 1431 | A |
| 1 | 5 | 1436 | A |
| 1 | 5 | 1446 | A |
| 1 | 5 | 1448 | A |
| 1 | 5 | 1452 | A |
| 1 | 5 | 1453 | A |
| 1 | 5 | 1455 | U |
| 1 | 5 | 1458 | G |
| 1 | 5 | 1466 | U |
| 1 | 5 | 1468 | C |
| 1 | 5 | 1471 | G |
| 1 | 5 | 1479 | C |
| 1 | 5 | 1496 | G |
| 1 | 5 | 1498 | C |
| 1 | 5 | 1499 | G |
| 1 | 5 | 1504 | U |
| 1 | 5 | 1507 | G |
| 1 | 5 | 1510 | A |
| 1 | 5 | 1513 | G |
| 1 | 5 | 1525 | U |
| 1 | 5 | 1526 | U |
| 1 | 5 | 1527 | C |
| 1 | 5 | 1528 | A |
| 1 | 5 | 1530 | A |
| 1 | 5 | 1531 | G |
| 1 | 5 | 1532 | G |
| 1 | 5 | 1533 | C |
| 1 | 5 | 1534 | C |
| 1 | 5 | 1536 | A |
| 1 | 5 | 1537 | A |
| 1 | 5 | 1539 | U |
| 1 | 5 | 1540 | U |
| 1 | 5 | 1542 | C |
| 1 | 5 | 1544 | A |
| 1 | 5 | 1545 | G |
| 1 | 5 | 1546 | G |
| 1 | 5 | 1547 | C |
| 1 | 5 | 1549 | A |
| 1 | 5 | 1550 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1551 | C |
| 1 | 5 | 1552 | A |
| 1 | 5 | 1555 | G |
| 1 | 5 | 1558 | A |
| 1 | 5 | 1559 | G |
| 1 | 5 | 1565 | C |
| 1 | 5 | 1576 | U |
| 1 | 5 | 1577 | C |
| 1 | 5 | 1584 | C |
| 1 | 5 | 1589 | U |
| 1 | 5 | 1597 | C |
| 1 | 5 | 1598 | U |
| 1 | 5 | 1599 | U |
| 1 | 5 | 1600 | C |
| 1 | 5 | 1601 | A |
| 1 | 5 | 1602 | C |
| 1 | 5 | 1608 | C |
| 1 | 5 | 1611 | A |
| 1 | 5 | 1612 | A |
| 1 | 5 | 1613 | C |
| 1 | 5 | 1614 | U |
| 1 | 5 | 1615 | G |
| 1 | 5 | 1624 | G |
| 1 | 5 | 1625 | A |
| 1 | 5 | 1627 | G |
| 1 | 5 | 1642 | G |
| 1 | 5 | 1644 | G |
| 1 | 5 | 1646 | G |
| 1 | 5 | 1652 | A |
| 1 | 5 | 1656 | U |
| 1 | 5 | 1657 | U |
| 1 | 5 | 1658 | U |
| 1 | 5 | 1671 | U |
| 1 | 5 | 1673 | A |
| 1 | 5 | 1684 | A |
| 1 | 5 | 1685 | U |
| 1 | 5 | 1686 | U |
| 1 | 5 | 1693 | U |
| 1 | 5 | 1694 | C |
| 1 | 5 | 1700 | A |
| 1 | 5 | 1710 | A |
| 1 | 5 | 1719 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1720 | G |
| 1 | 5 | 1725 | C |
| 1 | 5 | 1729 | C |
| 1 | 5 | 1731 | U |
| 1 | 5 | 1733 | G |
| 1 | 5 | 1734 | U |
| 1 | 5 | 1735 | G |
| 1 | 5 | 1739 | G |
| 1 | 5 | 1744 | G |
| 1 | 5 | 1747 | G |
| 1 | 5 | 1748 | C |
| 1 | 5 | 1749 | G |
| 1 | 5 | 1755 | G |
| 1 | 5 | 1763 | U |
| 1 | 5 | 1766 | A |
| 1 | 5 | 1777 | G |
| 1 | 5 | 1780 | G |
| 1 | 5 | 1781 | G |
| 1 | 5 | 1782 | A |
| 1 | 5 | 1783 | A |
| 1 | 5 | 1785 | A |
| 1 | 5 | 1786 | G |
| 1 | 5 | 1787 | U |
| 1 | 5 | 1789 | U |
| 1 | 5 | 1790 | U |
| 1 | 5 | 1792 | A |
| 1 | 5 | 1807 | G |
| 1 | 5 | 1808 | A |
| 1 | 5 | 1809 | U |
| 1 | 5 | 1810 | A |
| 1 | 5 | 1811 | A |
| 1 | 5 | 1815 | C |
| 1 | 5 | 1816 | A |
| 1 | 5 | 1818 | C |
| 1 | 5 | 1819 | A |
| 1 | 5 | 1823 | C |
| 1 | 5 | 1824 | U |
| 1 | 5 | 1828 | A |
| 1 | 5 | 1835 | C |
| 1 | 5 | 1836 | A |
| 1 | 5 | 1837 | G |
| 1 | 5 | 1840 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1845 | U |
| 1 | 5 | 1849 | U |
| 1 | 5 | 1850 | A |
| 1 | 5 | 1855 | A |
| 1 | 5 | 1859 | U |
| 1 | 5 | 1860 | A |
| 1 | 5 | 1862 | A |
| 1 | 5 | 1864 | A |
| 1 | 5 | 1865 | A |
| 1 | 5 | 1866 | G |
| 1 | 5 | 1870 | A |
| 1 | 5 | 1875 | G |
| 1 | 5 | 1878 | A |
| 1 | 5 | 1896 | G |
| 1 | 5 | 1917 | G |
| 1 | 5 | 1922 | G |
| 1 | 5 | 1923 | G |
| 1 | 5 | 1924 | C |
| 1 | 5 | 1925 | G |
| 1 | 5 | 1926 | U |
| 1 | 5 | 1928 | A |
| 1 | 5 | 1929 | G |
| 1 | 5 | 1941 | G |
| 1 | 5 | 1943 | C |
| 1 | 5 | 2025 | G |
| 1 | 5 | 2027 | C |
| 1 | 5 | 2032 | U |
| 1 | 5 | 2033 | U |
| 1 | 5 | 2036 | U |
| 1 | 5 | 2038 | G |
| 1 | 5 | 2041 | C |
| 1 | 5 | 2042 | U |
| 1 | 5 | 2046 | G |
| 1 | 5 | 2049 | G |
| 1 | 5 | 2050 | A |
| 1 | 5 | 2051 | U |
| 1 | 5 | 2052 | G |
| 1 | 5 | 2053 | C |
| 1 | 5 | 2054 | U |
| 1 | 5 | 2055 | G |
| 1 | 5 | 2057 | A |
| 1 | 5 | 2059 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2061 | A |
| 1 | 5 | 2062 | A |
| 1 | 5 | 2063 | C |
| 1 | 5 | 2064 | G |
| 1 | 5 | 2065 | A |
| 1 | 5 | 2069 | A |
| 1 | 5 | 2070 | C |
| 1 | 5 | 2071 | U |
| 1 | 5 | 2073 | A |
| 1 | 5 | 2080 | G |
| 1 | 5 | 2081 | U |
| 1 | 5 | 2082 | A |
| 1 | 5 | 2083 | C |
| 1 | 5 | 2087 | C |
| 1 | 5 | 2090 | G |
| 1 | 5 | 2091 | G |
| 1 | 5 | 2095 | A |
| 1 | 5 | 2100 | A |
| 1 | 5 | 2107 | A |
| 1 | 5 | 2108 | A |
| 1 | 5 | 2113 | A |
| 1 | 5 | 2114 | A |
| 1 | 5 | 2126 | G |
| 1 | 5 | 2127 | A |
| 1 | 5 | 2138 | G |
| 1 | 5 | 2139 | U |
| 1 | 5 | 2140 | G |
| 1 | 5 | 2155 | U |
| 1 | 5 | 2161 | C |
| 1 | 5 | 2165 | C |
| 1 | 5 | 2166 | C |
| 1 | 5 | 2169 | U |
| 1 | 5 | 2170 | G |
| 1 | 5 | 2173 | C |
| 1 | 5 | 2174 | U |
| 1 | 5 | 2175 | G |
| 1 | 5 | 2182 | A |
| 1 | 5 | 2191 | A |
| 1 | 5 | 2194 | U |
| 1 | 5 | 2198 | A |
| 1 | 5 | 2201 | A |
| 1 | 5 | 2213 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2217 | C |
| 1 | 5 | 2218 | G |
| 1 | 5 | 2219 | G |
| 1 | 5 | 2220 | G |
| 1 | 5 | 2221 | A |
| 1 | 5 | 2222 | G |
| 1 | 5 | 2223 | U |
| 1 | 5 | 2225 | A |
| 1 | 5 | 2226 | C |
| 1 | 5 | 2227 | U |
| 1 | 5 | 2228 | A |
| 1 | 5 | 2229 | U |
| 1 | 5 | 2230 | G |
| 1 | 5 | 2233 | U |
| 1 | 5 | 2235 | U |
| 1 | 5 | 2236 | C |
| 1 | 5 | 2237 | U |
| 1 | 5 | 2238 | U |
| 1 | 5 | 2239 | A |
| 1 | 5 | 2241 | G |
| 1 | 5 | 2242 | G |
| 1 | 5 | 2243 | U |
| 1 | 5 | 2245 | G |
| 1 | 5 | 2250 | A |
| 1 | 5 | 2251 | U |
| 1 | 5 | 2252 | G |
| 1 | 5 | 2257 | G |
| 1 | 5 | 2262 | C |
| 1 | 5 | 2263 | U |
| 1 | 5 | 2267 | U |
| 1 | 5 | 2275 | C |
| 1 | 5 | 2276 | G |
| 1 | 5 | 2277 | C |
| 1 | 5 | 2278 | A |
| 1 | 5 | 2279 | U |
| 1 | 5 | 2282 | A |
| 1 | 5 | 2284 | G |
| 1 | 5 | 2285 | G |
| 1 | 5 | 2288 | U |
| 1 | 5 | 2300 | C |
| 1 | 5 | 2301 | A |
| 1 | 5 | 2303 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2304 | G |
| 1 | 5 | 2305 | U |
| 1 | 5 | 2316 | U |
| 1 | 5 | 2336 | A |
| 1 | 5 | 2341 | A |
| 1 | 5 | 2342 | A |
| 1 | 5 | 2343 | C |
| 1 | 5 | 2344 | G |
| 1 | 5 | 2346 | G |
| 1 | 5 | 2347 | C |
| 1 | 5 | 2352 | C |
| 1 | 5 | 2354 | G |
| 1 | 5 | 2357 | U |
| 1 | 5 | 2358 | C |
| 1 | 5 | 2362 | G |
| 1 | 5 | 2366 | A |
| 1 | 5 | 2367 | A |
| 1 | 5 | 2369 | G |
| 1 | 5 | 2370 | A |
| 1 | 5 | 2371 | A |
| 1 | 5 | 2372 | G |
| 1 | 5 | 2373 | A |
| 1 | 5 | 2374 | C |
| 1 | 5 | 2380 | U |
| 1 | 5 | 2381 | G |
| 1 | 5 | 2387 | G |
| 1 | 5 | 2388 | A |
| 1 | 5 | 2390 | U |
| 1 | 5 | 2404 | G |
| 1 | 5 | 2407 | A |
| 1 | 5 | 2408 | A |
| 1 | 5 | 2412 | A |
| 1 | 5 | 2413 | C |
| 1 | 5 | 2414 | A |
| 1 | 5 | 2415 | U |
| 1 | 5 | 2416 | A |
| 1 | 5 | 2417 | G |
| 1 | 5 | 2418 | A |
| 1 | 5 | 2421 | G |
| 1 | 5 | 2422 | U |
| 1 | 5 | 2423 | G |
| 1 | 5 | 2427 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2428 | A |
| 1 | 5 | 2429 | U |
| 1 | 5 | 2430 | A |
| 1 | 5 | 2431 | A |
| 1 | 5 | 2432 | G |
| 1 | 5 | 2434 | G |
| 1 | 5 | 2438 | G |
| 1 | 5 | 2446 | G |
| 1 | 5 | 2451 | U |
| 1 | 5 | 2456 | U |
| 1 | 5 | 2457 | A |
| 1 | 5 | 2460 | A |
| 1 | 5 | 2461 | C |
| 1 | 5 | 2468 | U |
| 1 | 5 | 2469 | A |
| 1 | 5 | 2470 | U |
| 1 | 5 | 2471 | A |
| 1 | 5 | 2472 | G |
| 1 | 5 | 2473 | U |
| 1 | 5 | 2474 | U |
| 1 | 5 | 2475 | U |
| 1 | 5 | 2476 | C |
| 1 | 5 | 2479 | U |
| 1 | 5 | 2480 | A |
| 1 | 5 | 2481 | C |
| 1 | 5 | 2482 | U |
| 1 | 5 | 2483 | U |
| 1 | 5 | 2484 | A |
| 1 | 5 | 2491 | U |
| 1 | 5 | 2492 | A |
| 1 | 5 | 2493 | A |
| 1 | 5 | 2494 | G |
| 1 | 5 | 2495 | C |
| 1 | 5 | 2499 | G |
| 1 | 5 | 2500 | C |
| 1 | 5 | 2501 | U |
| 1 | 5 | 2502 | G |
| 1 | 5 | 2503 | G |
| 1 | 5 | 2506 | U |
| 1 | 5 | 2507 | U |
| 1 | 5 | 2508 | C |
| 1 | 5 | 2509 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2510 | U |
| 1 | 5 | 2511 | U |
| 1 | 5 | 2512 | U |
| 1 | 5 | 2517 | C |
| 1 | 5 | 2520 | U |
| 1 | 5 | 2521 | C |
| 1 | 5 | 2524 | G |
| 1 | 5 | 2526 | A |
| 1 | 5 | 2529 | C |
| 1 | 5 | 2530 | A |
| 1 | 5 | 2531 | A |
| 1 | 5 | 2537 | U |
| 1 | 5 | 2538 | A |
| 1 | 5 | 2540 | A |
| 1 | 5 | 2541 | C |
| 1 | 5 | 2542 | G |
| 1 | 5 | 2543 | G |
| 1 | 5 | 2547 | G |
| 1 | 5 | 2549 | U |
| 1 | 5 | 2553 | G |
| 1 | 5 | 2557 | G |
| 1 | 5 | 2561 | A |
| 1 | 5 | 2562 | C |
| 1 | 5 | 2568 | C |
| 1 | 5 | 2574 | G |
| 1 | 5 | 2575 | G |
| 1 | 5 | 2582 | G |
| 1 | 5 | 2587 | G |
| 1 | 5 | 2596 | A |
| 1 | 5 | 2604 | A |
| 1 | 5 | 2606 | C |
| 1 | 5 | 2609 | U |
| 1 | 5 | 2617 | A |
| 1 | 5 | 2620 | U |
| 1 | 5 | 2624 | A |
| 1 | 5 | 2625 | A |
| 1 | 5 | 2626 | G |
| 1 | 5 | 2630 | G |
| 1 | 5 | 2631 | A |
| 1 | 5 | 2635 | A |
| 1 | 5 | 2642 | A |
| 1 | 5 | 2646 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2647 | A |
| 1 | 5 | 2649 | U |
| 1 | 5 | 2657 | A |
| 1 | 5 | 2658 | G |
| 1 | 5 | 2659 | A |
| 1 | 5 | 2662 | A |
| 1 | 5 | 2664 | A |
| 1 | 5 | 2672 | A |
| 1 | 5 | 2682 | G |
| 1 | 5 | 2687 | U |
| 1 | 5 | 2688 | G |
| 1 | 5 | 2696 | G |
| 1 | 5 | 2697 | U |
| 1 | 5 | 2708 | A |
| 1 | 5 | 2715 | A |
| 1 | 5 | 2717 | G |
| 1 | 5 | 2720 | U |
| 1 | 5 | 2721 | G |
| 1 | 5 | 2722 | G |
| 1 | 5 | 2723 | C |
| 1 | 5 | 2726 | A |
| 1 | 5 | 2730 | A |
| 1 | 5 | 2739 | G |
| 1 | 5 | 2740 | U |
| 1 | 5 | 2741 | C |
| 1 | 5 | 2745 | G |
| 1 | 5 | 2746 | G |
| 1 | 5 | 2747 | A |
| 1 | 5 | 2764 | G |
| 1 | 5 | 2767 | A |
| 1 | 5 | 2768 | G |
| 1 | 5 | 2769 | A |
| 1 | 5 | 2770 | A |
| 1 | 5 | 2771 | A |
| 1 | 5 | 2778 | C |
| 1 | 5 | 2782 | G |
| 1 | 5 | 2784 | G |
| 1 | 5 | 2785 | A |
| 1 | 5 | 2786 | U |
| 1 | 5 | 2807 | G |
| 1 | 5 | 2811 | U |
| 1 | 5 | 2813 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2815 | A |
| 1 | 5 | 2818 | G |
| 1 | 5 | 2821 | A |
| 1 | 5 | 2824 | G |
| 1 | 5 | 2828 | U |
| 1 | 5 | 2829 | U |
| 1 | 5 | 2839 | G |
| 1 | 5 | 2840 | A |
| 1 | 5 | 2841 | U |
| 1 | 5 | 2843 | U |
| 1 | 5 | 2845 | G |
| 1 | 5 | 2848 | U |
| 1 | 5 | 2855 | A |
| 1 | 5 | 2857 | C |
| 1 | 5 | 2860 | A |
| 1 | 5 | 2864 | A |
| 1 | 5 | 2866 | G |
| 1 | 5 | 2867 | C |
| 1 | 5 | 2869 | G |
| 1 | 5 | 2872 | U |
| 1 | 5 | 2878 | A |
| 1 | 5 | 2880 | G |
| 1 | 5 | 2882 | G |
| 1 | 5 | 2886 | G |
| 1 | 5 | 2890 | G |
| 1 | 5 | 2891 | U |
| 1 | 5 | 2895 | C |
| 1 | 5 | 2903 | U |
| 1 | 5 | 2904 | A |
| 1 | 5 | 2906 | G |
| 1 | 5 | 2910 | C |
| 1 | 5 | 2915 | G |
| 1 | 5 | 2922 | U |
| 1 | 5 | 2923 | U |
| 1 | 5 | 2925 | G |
| 1 | 5 | 2936 | G |
| 1 | 5 | 2939 | A |
| 1 | 5 | 2940 | G |
| 1 | 5 | 2947 | U |
| 1 | 5 | 2948 | U |
| 1 | 5 | 2951 | C |
| 1 | 5 | 2955 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2958 | G |
| 1 | 5 | 2964 | U |
| 1 | 5 | 2965 | G |
| 1 | 5 | 2980 | A |
| 1 | 5 | 2989 | A |
| 1 | 5 | 2991 | U |
| 1 | 5 | 2996 | G |
| 1 | 5 | 2998 | G |
| 1 | 5 | 3008 | A |
| 1 | 5 | 3017 | A |
| 1 | 5 | 3023 | U |
| 1 | 5 | 3024 | U |
| 1 | 5 | 3025 | U |
| 1 | 5 | 3026 | U |
| 1 | 5 | 3027 | G |
| 1 | 5 | 3040 | C |
| 1 | 5 | 3041 | A |
| 1 | 5 | 3042 | G |
| 1 | 5 | 3046 | U |
| 1 | 5 | 3047 | U |
| 1 | 5 | 3048 | G |
| 1 | 5 | 3054 | A |
| 1 | 5 | 3055 | A |
| 1 | 5 | 3059 | A |
| 1 | 5 | 3060 | C |
| 1 | 5 | 3062 | A |
| 1 | 5 | 3069 | G |
| 1 | 5 | 3072 | U |
| 1 | 5 | 3077 | G |
| 1 | 5 | 3083 | C |
| 1 | 5 | 3090 | A |
| 1 | 5 | 3093 | U |
| 1 | 5 | 3098 | A |
| 1 | 5 | 3099 | U |
| 1 | 5 | 3110 | A |
| 1 | 5 | 3113 | C |
| 1 | 5 | 3119 | U |
| 1 | 5 | 3121 | U |
| 1 | 5 | 3122 | C |
| 1 | 5 | 3123 | U |
| 1 | 5 | 3124 | U |
| 1 | 5 | 3125 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 3126 | G |
| 1 | 5 | 3133 | A |
| 1 | 5 | 3136 | A |
| 1 | 5 | 3138 | A |
| 1 | 5 | 3139 | U |
| 1 | 5 | 3140 | A |
| 1 | 5 | 3141 | G |
| 1 | 5 | 3142 | A |
| 1 | 5 | 3143 | A |
| 1 | 5 | 3144 | G |
| 1 | 5 | 3147 | U |
| 1 | 5 | 3149 | A |
| 1 | 5 | 3152 | A |
| 1 | 5 | 3155 | A |
| 1 | 5 | 3161 | C |
| 1 | 5 | 3163 | U |
| 1 | 5 | 3164 | U |
| 1 | 5 | 3165 | U |
| 1 | 5 | 3175 | U |
| 1 | 5 | 3176 | G |
| 1 | 5 | 3185 | C |
| 1 | 5 | 3186 | A |
| 1 | 5 | 3187 | G |
| 1 | 5 | 3188 | G |
| 1 | 5 | 3195 | A |
| 1 | 5 | 3197 | G |
| 1 | 5 | 3203 | C |
| 1 | 5 | 3206 | A |
| 1 | 5 | 3207 | G |
| 1 | 5 | 3208 | C |
| 1 | 5 | 3210 | G |
| 1 | 5 | 3211 | A |
| 1 | 5 | 3212 | A |
| 1 | 5 | 3213 | A |
| 1 | 5 | 3214 | G |
| 1 | 5 | 3215 | G |
| 1 | 5 | 3217 | U |
| 1 | 5 | 3220 | G |
| 1 | 5 | 3221 | G |
| 1 | 5 | 3227 | U |
| 1 | 5 | 3231 | G |
| 1 | 5 | 3233 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 3236 | A |
| 1 | 5 | 3238 | U |
| 1 | 5 | 3241 | A |
| 1 | 5 | 3243 | U |
| 1 | 5 | 3244 | G |
| 1 | 5 | 3245 | U |
| 1 | 5 | 3246 | C |
| 1 | 5 | 3247 | A |
| 1 | 5 | 3249 | U |
| 1 | 5 | 3250 | U |
| 1 | 5 | 3253 | C |
| 1 | 5 | 3254 | G |
| 1 | 5 | 3257 | A |
| 1 | 5 | 3258 | G |
| 1 | 5 | 3262 | A |
| 1 | 5 | 3263 | A |
| 1 | 5 | 3272 | U |
| 1 | 5 | 3273 | A |
| 1 | 5 | 3275 | A |
| 1 | 5 | 3281 | U |
| 1 | 5 | 3284 | A |
| 1 | 5 | 3285 | U |
| 1 | 5 | 3286 | G |
| 1 | 5 | 3287 | U |
| 1 | 5 | 3291 | A |
| 1 | 5 | 3299 | U |
| 1 | 5 | 3303 | A |
| 1 | 5 | 3309 | U |
| 1 | 5 | 3310 | A |
| 1 | 5 | 3313 | G |
| 1 | 5 | 3316 | G |
| 1 | 5 | 3319 | U |
| 1 | 5 | 3322 | U |
| 1 | 5 | 3324 | G |
| 1 | 5 | 3326 | U |
| 1 | 5 | 3336 | U |
| 1 | 5 | 3337 | G |
| 1 | 5 | 3346 | C |
| 1 | 5 | 3350 | C |
| 1 | 5 | 3351 | G |
| 1 | 5 | 3354 | G |
| 1 | 5 | 3357 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 3358 | G |
| 1 | 5 | 3360 | U |
| 1 | 5 | 3364 | U |
| 2 | 7 | 6 | C |
| 2 | 7 | 13 | A |
| 2 | 7 | 22 | A |
| 2 | 7 | 38 | U |
| 2 | 7 | 41 | G |
| 2 | 7 | 50 | U |
| 2 | 7 | 51 | A |
| 2 | 7 | 52 | G |
| 2 | 7 | 54 | U |
| 2 | 7 | 65 | G |
| 2 | 7 | 73 | C |
| 2 | 7 | 74 | C |
| 2 | 7 | 76 | A |
| 2 | 7 | 77 | G |
| 2 | 7 | 91 | G |
| 2 | 7 | 93 | C |
| 2 | 7 | 99 | G |
| 2 | 7 | 101 | G |
| 2 | 7 | 102 | A |
| 2 | 7 | 104 | A |
| 2 | 7 | 112 | G |
| 2 | 7 | 121 | U |
| 3 | 8 | 2 | A |
| 3 | 8 | 7 | U |
| 3 | 8 | 8 | C |
| 3 | 8 | 13 | A |
| 3 | 8 | 21 | C |
| 3 | 8 | 23 | U |
| 3 | 8 | 25 | G |
| 3 | 8 | 34 | U |
| 3 | 8 | 35 | C |
| 3 | 8 | 38 | U |
| 3 | 8 | 47 | C |
| 3 | 8 | 48 | A |
| 3 | 8 | 51 | G |
| 3 | 8 | 59 | A |
| 3 | 8 | 62 | U |
| 3 | 8 | 63 | G |
| 3 | 8 | 79 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 8 | 81 | U |
| 3 | 8 | 84 | C |
| 3 | 8 | 86 | U |
| 3 | 8 | 87 | G |
| 3 | 8 | 90 | U |
| 3 | 8 | 91 | C |
| 3 | 8 | 95 | A |
| 3 | 8 | 97 | A |
| 3 | 8 | 100 | U |
| 3 | 8 | 104 | A |
| 3 | 8 | 105 | A |
| 3 | 8 | 106 | C |
| 3 | 8 | 108 | C |
| 3 | 8 | 111 | A |
| 3 | 8 | 113 | U |
| 3 | 8 | 116 | G |
| 3 | 8 | 125 | U |
| 3 | 8 | 126 | A |
| 3 | 8 | 127 | U |
| 3 | 8 | 129 | C |
| 3 | 8 | 144 | G |
| 3 | 8 | 156 | U |
| 3 | 8 | 157 | U |
| 81 | 2 | 2 | A |
| 81 | 2 | 3 | U |
| 81 | 2 | 4 | C |
| 81 | 2 | 5 | U |
| 81 | 2 | 8 | U |
| 81 | 2 | 9 | U |
| 81 | 2 | 10 | G |
| 81 | 2 | 11 | A |
| 81 | 2 | 14 | C |
| 81 | 2 | 17 | C |
| 81 | 2 | 22 | A |
| 81 | 2 | 23 | G |
| 81 | 2 | 25 | C |
| 81 | 2 | 26 | A |
| 81 | 2 | 29 | U |
| 81 | 2 | 31 | C |
| 81 | 2 | 32 | U |
| 81 | 2 | 34 | G |
| 81 | 2 | 40 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 42 | G |
| 81 | 2 | 45 | U |
| 81 | 2 | 47 | A |
| 81 | 2 | 50 | C |
| 81 | 2 | 51 | A |
| 81 | 2 | 57 | G |
| 81 | 2 | 58 | U |
| 81 | 2 | 61 | A |
| 81 | 2 | 62 | A |
| 81 | 2 | 63 | G |
| 81 | 2 | 64 | U |
| 81 | 2 | 65 | A |
| 81 | 2 | 67 | A |
| 81 | 2 | 68 | A |
| 81 | 2 | 69 | G |
| 81 | 2 | 71 | A |
| 81 | 2 | 72 | A |
| 81 | 2 | 73 | U |
| 81 | 2 | 74 | U |
| 81 | 2 | 75 | U |
| 81 | 2 | 76 | A |
| 81 | 2 | 77 | U |
| 81 | 2 | 78 | A |
| 81 | 2 | 80 | A |
| 81 | 2 | 81 | G |
| 81 | 2 | 93 | A |
| 81 | 2 | 104 | A |
| 81 | 2 | 107 | C |
| 81 | 2 | 111 | U |
| 81 | 2 | 113 | U |
| 81 | 2 | 114 | C |
| 81 | 2 | 115 | G |
| 81 | 2 | 124 | A |
| 81 | 2 | 125 | U |
| 81 | 2 | 126 | A |
| 81 | 2 | 127 | G |
| 81 | 2 | 129 | U |
| 81 | 2 | 130 | C |
| 81 | 2 | 131 | C |
| 81 | 2 | 132 | U |
| 81 | 2 | 133 | U |
| 81 | 2 | 134 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 136 | C |
| 81 | 2 | 137 | U |
| 81 | 2 | 138 | A |
| 81 | 2 | 139 | C |
| 81 | 2 | 140 | A |
| 81 | 2 | 146 | A |
| 81 | 2 | 147 | U |
| 81 | 2 | 149 | U |
| 81 | 2 | 150 | G |
| 81 | 2 | 152 | G |
| 81 | 2 | 154 | U |
| 81 | 2 | 155 | A |
| 81 | 2 | 156 | A |
| 81 | 2 | 158 | U |
| 81 | 2 | 159 | C |
| 81 | 2 | 160 | U |
| 81 | 2 | 161 | A |
| 81 | 2 | 165 | C |
| 81 | 2 | 166 | U |
| 81 | 2 | 167 | A |
| 81 | 2 | 169 | U |
| 81 | 2 | 170 | A |
| 81 | 2 | 173 | U |
| 81 | 2 | 175 | C |
| 81 | 2 | 176 | U |
| 81 | 2 | 177 | U |
| 81 | 2 | 178 | A |
| 81 | 2 | 180 | A |
| 81 | 2 | 183 | C |
| 81 | 2 | 184 | U |
| 81 | 2 | 186 | G |
| 81 | 2 | 187 | A |
| 81 | 2 | 190 | C |
| 81 | 2 | 191 | U |
| 81 | 2 | 192 | U |
| 81 | 2 | 194 | G |
| 81 | 2 | 198 | G |
| 81 | 2 | 199 | A |
| 81 | 2 | 203 | G |
| 81 | 2 | 205 | A |
| 81 | 2 | 209 | A |
| 81 | 2 | 217 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 218 | A |
| 81 | 2 | 220 | A |
| 81 | 2 | 224 | A |
| 81 | 2 | 225 | A |
| 81 | 2 | 226 | U |
| 81 | 2 | 228 | U |
| 81 | 2 | 230 | U |
| 81 | 2 | 232 | C |
| 81 | 2 | 233 | G |
| 81 | 2 | 234 | G |
| 81 | 2 | 239 | C |
| 81 | 2 | 240 | U |
| 81 | 2 | 241 | U |
| 81 | 2 | 249 | C |
| 81 | 2 | 253 | A |
| 81 | 2 | 256 | A |
| 81 | 2 | 259 | U |
| 81 | 2 | 260 | U |
| 81 | 2 | 264 | A |
| 81 | 2 | 265 | A |
| 81 | 2 | 266 | U |
| 81 | 2 | 274 | C |
| 81 | 2 | 275 | C |
| 81 | 2 | 276 | U |
| 81 | 2 | 277 | U |
| 81 | 2 | 278 | G |
| 81 | 2 | 279 | U |
| 81 | 2 | 280 | G |
| 81 | 2 | 286 | G |
| 81 | 2 | 288 | U |
| 81 | 2 | 289 | G |
| 81 | 2 | 294 | A |
| 81 | 2 | 298 | A |
| 81 | 2 | 301 | U |
| 81 | 2 | 305 | U |
| 81 | 2 | 308 | C |
| 81 | 2 | 311 | A |
| 81 | 2 | 312 | U |
| 81 | 2 | 313 | C |
| 81 | 2 | 314 | A |
| 81 | 2 | 315 | A |
| 81 | 2 | 319 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 320 | C |
| 81 | 2 | 321 | G |
| 81 | 2 | 322 | A |
| 81 | 2 | 328 | G |
| 81 | 2 | 332 | A |
| 81 | 2 | 334 | U |
| 81 | 2 | 335 | G |
| 81 | 2 | 336 | G |
| 81 | 2 | 337 | C |
| 81 | 2 | 349 | U |
| 81 | 2 | 350 | C |
| 81 | 2 | 351 | A |
| 81 | 2 | 358 | A |
| 81 | 2 | 359 | A |
| 81 | 2 | 360 | C |
| 81 | 2 | 361 | G |
| 81 | 2 | 368 | A |
| 81 | 2 | 369 | A |
| 81 | 2 | 370 | G |
| 81 | 2 | 372 | G |
| 81 | 2 | 373 | U |
| 81 | 2 | 377 | A |
| 81 | 2 | 380 | C |
| 81 | 2 | 384 | A |
| 81 | 2 | 385 | G |
| 81 | 2 | 386 | A |
| 81 | 2 | 387 | G |
| 81 | 2 | 389 | G |
| 81 | 2 | 392 | C |
| 81 | 2 | 397 | G |
| 81 | 2 | 399 | A |
| 81 | 2 | 400 | A |
| 81 | 2 | 401 | C |
| 81 | 2 | 403 | G |
| 81 | 2 | 408 | C |
| 81 | 2 | 411 | A |
| 81 | 2 | 412 | U |
| 81 | 2 | 414 | C |
| 81 | 2 | 415 | A |
| 81 | 2 | 416 | A |
| 81 | 2 | 417 | G |
| 81 | 2 | 418 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 421 | G |
| 81 | 2 | 423 | C |
| 81 | 2 | 424 | A |
| 81 | 2 | 425 | G |
| 81 | 2 | 433 | G |
| 81 | 2 | 436 | A |
| 81 | 2 | 438 | U |
| 81 | 2 | 439 | U |
| 81 | 2 | 440 | A |
| 81 | 2 | 443 | C |
| 81 | 2 | 444 | A |
| 81 | 2 | 447 | C |
| 81 | 2 | 452 | U |
| 81 | 2 | 453 | U |
| 81 | 2 | 454 | C |
| 81 | 2 | 455 | A |
| 81 | 2 | 458 | G |
| 81 | 2 | 459 | A |
| 81 | 2 | 460 | G |
| 81 | 2 | 463 | A |
| 81 | 2 | 467 | A |
| 81 | 2 | 468 | C |
| 81 | 2 | 474 | A |
| 81 | 2 | 475 | U |
| 81 | 2 | 476 | A |
| 81 | 2 | 479 | G |
| 81 | 2 | 480 | A |
| 81 | 2 | 483 | C |
| 81 | 2 | 490 | C |
| 81 | 2 | 491 | A |
| 81 | 2 | 492 | U |
| 81 | 2 | 493 | U |
| 81 | 2 | 494 | C |
| 81 | 2 | 497 | G |
| 81 | 2 | 499 | C |
| 81 | 2 | 500 | U |
| 81 | 2 | 503 | U |
| 81 | 2 | 504 | A |
| 81 | 2 | 505 | A |
| 81 | 2 | 506 | U |
| 81 | 2 | 507 | U |
| 81 | 2 | 509 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 510 | A |
| 81 | 2 | 511 | A |
| 81 | 2 | 512 | U |
| 81 | 2 | 513 | G |
| 81 | 2 | 514 | A |
| 81 | 2 | 515 | G |
| 81 | 2 | 518 | C |
| 81 | 2 | 519 | A |
| 81 | 2 | 526 | A |
| 81 | 2 | 527 | U |
| 81 | 2 | 530 | C |
| 81 | 2 | 533 | A |
| 81 | 2 | 534 | A |
| 81 | 2 | 535 | C |
| 81 | 2 | 537 | A |
| 81 | 2 | 539 | G |
| 81 | 2 | 540 | A |
| 81 | 2 | 541 | A |
| 81 | 2 | 542 | C |
| 81 | 2 | 543 | A |
| 81 | 2 | 544 | A |
| 81 | 2 | 545 | C |
| 81 | 2 | 547 | G |
| 81 | 2 | 548 | G |
| 81 | 2 | 553 | C |
| 81 | 2 | 554 | A |
| 81 | 2 | 556 | G |
| 81 | 2 | 557 | U |
| 81 | 2 | 558 | C |
| 81 | 2 | 559 | U |
| 81 | 2 | 560 | G |
| 81 | 2 | 563 | G |
| 81 | 2 | 565 | C |
| 81 | 2 | 567 | G |
| 81 | 2 | 570 | G |
| 81 | 2 | 571 | C |
| 81 | 2 | 573 | G |
| 81 | 2 | 574 | C |
| 81 | 2 | 576 | G |
| 81 | 2 | 577 | U |
| 81 | 2 | 578 | A |
| 81 | 2 | 579 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 581 | U |
| 81 | 2 | 582 | C |
| 81 | 2 | 593 | A |
| 81 | 2 | 594 | G |
| 81 | 2 | 596 | G |
| 81 | 2 | 600 | A |
| 81 | 2 | 605 | A |
| 81 | 2 | 606 | G |
| 81 | 2 | 607 | U |
| 81 | 2 | 609 | G |
| 81 | 2 | 610 | U |
| 81 | 2 | 613 | C |
| 81 | 2 | 615 | G |
| 81 | 2 | 618 | A |
| 81 | 2 | 619 | A |
| 81 | 2 | 622 | A |
| 81 | 2 | 623 | G |
| 81 | 2 | 634 | A |
| 81 | 2 | 637 | U |
| 81 | 2 | 638 | U |
| 81 | 2 | 639 | U |
| 81 | 2 | 640 | G |
| 81 | 2 | 642 | G |
| 81 | 2 | 647 | G |
| 81 | 2 | 648 | U |
| 81 | 2 | 649 | U |
| 81 | 2 | 652 | C |
| 81 | 2 | 653 | C |
| 81 | 2 | 654 | G |
| 81 | 2 | 655 | G |
| 81 | 2 | 677 | G |
| 81 | 2 | 678 | U |
| 81 | 2 | 679 | U |
| 81 | 2 | 683 | C |
| 81 | 2 | 684 | A |
| 81 | 2 | 691 | U |
| 81 | 2 | 694 | U |
| 81 | 2 | 695 | U |
| 81 | 2 | 696 | C |
| 81 | 2 | 697 | C |
| 81 | 2 | 698 | U |
| 81 | 2 | 701 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 704 | C |
| 81 | 2 | 705 | U |
| 81 | 2 | 708 | C |
| 81 | 2 | 709 | C |
| 81 | 2 | 710 | U |
| 81 | 2 | 711 | G |
| 81 | 2 | 712 | U |
| 81 | 2 | 714 | C |
| 81 | 2 | 716 | C |
| 81 | 2 | 717 | C |
| 81 | 2 | 718 | U |
| 81 | 2 | 719 | U |
| 81 | 2 | 722 | G |
| 81 | 2 | 724 | G |
| 81 | 2 | 727 | C |
| 81 | 2 | 731 | C |
| 81 | 2 | 732 | G |
| 81 | 2 | 733 | A |
| 81 | 2 | 734 | A |
| 81 | 2 | 735 | C |
| 81 | 2 | 736 | C |
| 81 | 2 | 737 | A |
| 81 | 2 | 738 | G |
| 81 | 2 | 740 | A |
| 81 | 2 | 741 | C |
| 81 | 2 | 742 | U |
| 81 | 2 | 743 | U |
| 81 | 2 | 745 | U |
| 81 | 2 | 753 | A |
| 81 | 2 | 754 | A |
| 81 | 2 | 765 | G |
| 81 | 2 | 766 | U |
| 81 | 2 | 767 | U |
| 81 | 2 | 769 | A |
| 81 | 2 | 771 | A |
| 81 | 2 | 774 | A |
| 81 | 2 | 778 | G |
| 81 | 2 | 779 | A |
| 81 | 2 | 780 | A |
| 81 | 2 | 781 | A |
| 81 | 2 | 782 | G |
| 81 | 2 | 785 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 786 | G |
| 81 | 2 | 787 | A |
| 81 | 2 | 788 | A |
| 81 | 2 | 789 | U |
| 81 | 2 | 791 | U |
| 81 | 2 | 792 | A |
| 81 | 2 | 793 | U |
| 81 | 2 | 794 | U |
| 81 | 2 | 795 | A |
| 81 | 2 | 800 | G |
| 81 | 2 | 802 | A |
| 81 | 2 | 809 | G |
| 81 | 2 | 810 | A |
| 81 | 2 | 811 | A |
| 81 | 2 | 812 | U |
| 81 | 2 | 813 | A |
| 81 | 2 | 814 | G |
| 81 | 2 | 815 | G |
| 81 | 2 | 817 | C |
| 81 | 2 | 819 | U |
| 81 | 2 | 820 | U |
| 81 | 2 | 821 | U |
| 81 | 2 | 822 | G |
| 81 | 2 | 823 | G |
| 81 | 2 | 825 | U |
| 81 | 2 | 826 | C |
| 81 | 2 | 828 | A |
| 81 | 2 | 829 | U |
| 81 | 2 | 830 | U |
| 81 | 2 | 831 | U |
| 81 | 2 | 832 | U |
| 81 | 2 | 834 | U |
| 81 | 2 | 837 | G |
| 81 | 2 | 840 | U |
| 81 | 2 | 842 | U |
| 81 | 2 | 845 | G |
| 81 | 2 | 848 | C |
| 81 | 2 | 849 | A |
| 81 | 2 | 851 | C |
| 81 | 2 | 852 | G |
| 81 | 2 | 855 | A |
| 81 | 2 | 859 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 860 | U |
| 81 | 2 | 862 | A |
| 81 | 2 | 863 | U |
| 81 | 2 | 872 | U |
| 81 | 2 | 875 | G |
| 81 | 2 | 876 | G |
| 81 | 2 | 884 | G |
| 81 | 2 | 885 | U |
| 81 | 2 | 886 | A |
| 81 | 2 | 887 | U |
| 81 | 2 | 895 | U |
| 81 | 2 | 897 | A |
| 81 | 2 | 903 | G |
| 81 | 2 | 904 | A |
| 81 | 2 | 905 | A |
| 81 | 2 | 906 | A |
| 81 | 2 | 908 | U |
| 81 | 2 | 909 | C |
| 81 | 2 | 910 | U |
| 81 | 2 | 912 | G |
| 81 | 2 | 913 | G |
| 81 | 2 | 914 | A |
| 81 | 2 | 915 | U |
| 81 | 2 | 916 | U |
| 81 | 2 | 920 | U |
| 81 | 2 | 922 | A |
| 81 | 2 | 926 | C |
| 81 | 2 | 927 | U |
| 81 | 2 | 928 | A |
| 81 | 2 | 929 | A |
| 81 | 2 | 930 | C |
| 81 | 2 | 931 | U |
| 81 | 2 | 932 | A |
| 81 | 2 | 934 | U |
| 81 | 2 | 938 | A |
| 81 | 2 | 939 | A |
| 81 | 2 | 943 | A |
| 81 | 2 | 950 | A |
| 81 | 2 | 958 | U |
| 81 | 2 | 959 | U |
| 81 | 2 | 964 | U |
| 81 | 2 | 965 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 969 | A |
| 81 | 2 | 972 | A |
| 81 | 2 | 980 | U |
| 81 | 2 | 981 | U |
| 81 | 2 | 982 | A |
| 81 | 2 | 983 | G |
| 81 | 2 | 985 | G |
| 81 | 2 | 987 | A |
| 81 | 2 | 990 | G |
| 81 | 2 | 991 | A |
| 81 | 2 | 992 | A |
| 81 | 2 | 993 | G |
| 81 | 2 | 999 | C |
| 81 | 2 | 1001 | G |
| 81 | 2 | 1002 | A |
| 81 | 2 | 1003 | U |
| 81 | 2 | 1004 | A |
| 81 | 2 | 1005 | C |
| 81 | 2 | 1009 | C |
| 81 | 2 | 1010 | G |
| 81 | 2 | 1011 | U |
| 81 | 2 | 1012 | A |
| 81 | 2 | 1013 | G |
| 81 | 2 | 1015 | C |
| 81 | 2 | 1018 | A |
| 81 | 2 | 1020 | C |
| 81 | 2 | 1024 | A |
| 81 | 2 | 1025 | A |
| 81 | 2 | 1026 | A |
| 81 | 2 | 1027 | C |
| 81 | 2 | 1028 | U |
| 81 | 2 | 1030 | U |
| 81 | 2 | 1031 | G |
| 81 | 2 | 1033 | C |
| 81 | 2 | 1035 | A |
| 81 | 2 | 1037 | U |
| 81 | 2 | 1038 | A |
| 81 | 2 | 1039 | G |
| 81 | 2 | 1041 | G |
| 81 | 2 | 1042 | A |
| 81 | 2 | 1044 | C |
| 81 | 2 | 1045 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1048 | U |
| 81 | 2 | 1050 | G |
| 81 | 2 | 1051 | U |
| 81 | 2 | 1052 | G |
| 81 | 2 | 1056 | U |
| 81 | 2 | 1057 | U |
| 81 | 2 | 1058 | C |
| 81 | 2 | 1059 | U |
| 81 | 2 | 1060 | U |
| 81 | 2 | 1063 | G |
| 81 | 2 | 1070 | U |
| 81 | 2 | 1071 | C |
| 81 | 2 | 1080 | A |
| 81 | 2 | 1081 | C |
| 81 | 2 | 1082 | G |
| 81 | 2 | 1083 | A |
| 81 | 2 | 1087 | A |
| 81 | 2 | 1090 | A |
| 81 | 2 | 1091 | A |
| 81 | 2 | 1092 | A |
| 81 | 2 | 1093 | G |
| 81 | 2 | 1094 | U |
| 81 | 2 | 1096 | U |
| 81 | 2 | 1097 | U |
| 81 | 2 | 1098 | U |
| 81 | 2 | 1099 | G |
| 81 | 2 | 1100 | G |
| 81 | 2 | 1102 | U |
| 81 | 2 | 1103 | U |
| 81 | 2 | 1104 | C |
| 81 | 2 | 1107 | G |
| 81 | 2 | 1108 | G |
| 81 | 2 | 1110 | G |
| 81 | 2 | 1113 | G |
| 81 | 2 | 1118 | G |
| 81 | 2 | 1121 | G |
| 81 | 2 | 1130 | A |
| 81 | 2 | 1137 | A |
| 81 | 2 | 1139 | G |
| 81 | 2 | 1142 | A |
| 81 | 2 | 1145 | G |
| 81 | 2 | 1149 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1150 | A |
| 81 | 2 | 1157 | C |
| 81 | 2 | 1158 | C |
| 81 | 2 | 1159 | A |
| 81 | 2 | 1162 | A |
| 81 | 2 | 1166 | G |
| 81 | 2 | 1184 | U |
| 81 | 2 | 1185 | U |
| 81 | 2 | 1193 | A |
| 81 | 2 | 1195 | A |
| 81 | 2 | 1196 | C |
| 81 | 2 | 1198 | G |
| 81 | 2 | 1199 | G |
| 81 | 2 | 1201 | A |
| 81 | 2 | 1202 | A |
| 81 | 2 | 1203 | A |
| 81 | 2 | 1204 | C |
| 81 | 2 | 1212 | G |
| 81 | 2 | 1213 | U |
| 81 | 2 | 1216 | A |
| 81 | 2 | 1217 | G |
| 81 | 2 | 1218 | A |
| 81 | 2 | 1219 | C |
| 81 | 2 | 1222 | A |
| 81 | 2 | 1226 | A |
| 81 | 2 | 1227 | G |
| 81 | 2 | 1228 | G |
| 81 | 2 | 1229 | A |
| 81 | 2 | 1230 | U |
| 81 | 2 | 1234 | C |
| 81 | 2 | 1236 | G |
| 81 | 2 | 1238 | U |
| 81 | 2 | 1240 | G |
| 81 | 2 | 1241 | A |
| 81 | 2 | 1242 | G |
| 81 | 2 | 1243 | A |
| 81 | 2 | 1244 | G |
| 81 | 2 | 1245 | C |
| 81 | 2 | 1247 | C |
| 81 | 2 | 1250 | U |
| 81 | 2 | 1253 | U |
| 81 | 2 | 1254 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1258 | U |
| 81 | 2 | 1259 | U |
| 81 | 2 | 1265 | U |
| 81 | 2 | 1268 | U |
| 81 | 2 | 1269 | G |
| 81 | 2 | 1272 | G |
| 81 | 2 | 1274 | A |
| 81 | 2 | 1282 | U |
| 81 | 2 | 1284 | U |
| 81 | 2 | 1292 | U |
| 81 | 2 | 1294 | G |
| 81 | 2 | 1296 | G |
| 81 | 2 | 1300 | U |
| 81 | 2 | 1306 | U |
| 81 | 2 | 1310 | U |
| 81 | 2 | 1311 | A |
| 81 | 2 | 1313 | U |
| 81 | 2 | 1314 | U |
| 81 | 2 | 1315 | G |
| 81 | 2 | 1316 | C |
| 81 | 2 | 1319 | U |
| 81 | 2 | 1320 | A |
| 81 | 2 | 1321 | A |
| 81 | 2 | 1322 | C |
| 81 | 2 | 1324 | A |
| 81 | 2 | 1336 | A |
| 81 | 2 | 1337 | C |
| 81 | 2 | 1339 | U |
| 81 | 2 | 1340 | A |
| 81 | 2 | 1343 | A |
| 81 | 2 | 1344 | A |
| 81 | 2 | 1345 | A |
| 81 | 2 | 1347 | A |
| 81 | 2 | 1349 | G |
| 81 | 2 | 1353 | G |
| 81 | 2 | 1356 | G |
| 81 | 2 | 1358 | C |
| 81 | 2 | 1359 | A |
| 81 | 2 | 1360 | C |
| 81 | 2 | 1361 | U |
| 81 | 2 | 1362 | U |
| 81 | 2 | 1363 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1364 | C |
| 81 | 2 | 1366 | G |
| 81 | 2 | 1369 | U |
| 81 | 2 | 1370 | G |
| 81 | 2 | 1371 | A |
| 81 | 2 | 1380 | A |
| 81 | 2 | 1386 | A |
| 81 | 2 | 1387 | C |
| 81 | 2 | 1388 | U |
| 81 | 2 | 1393 | G |
| 81 | 2 | 1396 | U |
| 81 | 2 | 1397 | C |
| 81 | 2 | 1398 | A |
| 81 | 2 | 1400 | G |
| 81 | 2 | 1410 | G |
| 81 | 2 | 1411 | U |
| 81 | 2 | 1412 | U |
| 81 | 2 | 1413 | U |
| 81 | 2 | 1416 | G |
| 81 | 2 | 1417 | G |
| 81 | 2 | 1423 | A |
| 81 | 2 | 1425 | A |
| 81 | 2 | 1426 | G |
| 81 | 2 | 1429 | C |
| 81 | 2 | 1430 | U |
| 81 | 2 | 1432 | U |
| 81 | 2 | 1433 | G |
| 81 | 2 | 1434 | A |
| 81 | 2 | 1438 | C |
| 81 | 2 | 1439 | C |
| 81 | 2 | 1442 | A |
| 81 | 2 | 1443 | G |
| 81 | 2 | 1444 | A |
| 81 | 2 | 1445 | C |
| 81 | 2 | 1446 | G |
| 81 | 2 | 1447 | U |
| 81 | 2 | 1449 | C |
| 81 | 2 | 1450 | U |
| 81 | 2 | 1452 | G |
| 81 | 2 | 1454 | C |
| 81 | 2 | 1455 | C |
| 81 | 2 | 1456 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1457 | C |
| 81 | 2 | 1458 | A |
| 81 | 2 | 1459 | C |
| 81 | 2 | 1461 | C |
| 81 | 2 | 1464 | G |
| 81 | 2 | 1467 | A |
| 81 | 2 | 1468 | C |
| 81 | 2 | 1469 | A |
| 81 | 2 | 1470 | C |
| 81 | 2 | 1471 | U |
| 81 | 2 | 1475 | G |
| 81 | 2 | 1476 | G |
| 81 | 2 | 1481 | A |
| 81 | 2 | 1484 | G |
| 81 | 2 | 1485 | A |
| 81 | 2 | 1487 | U |
| 81 | 2 | 1488 | A |
| 81 | 2 | 1489 | C |
| 81 | 2 | 1490 | A |
| 81 | 2 | 1491 | A |
| 81 | 2 | 1492 | C |
| 81 | 2 | 1494 | U |
| 81 | 2 | 1495 | U |
| 81 | 2 | 1498 | C |
| 81 | 2 | 1502 | G |
| 81 | 2 | 1506 | U |
| 81 | 2 | 1507 | C |
| 81 | 2 | 1508 | U |
| 81 | 2 | 1509 | G |
| 81 | 2 | 1512 | U |
| 81 | 2 | 1513 | A |
| 81 | 2 | 1514 | A |
| 81 | 2 | 1515 | U |
| 81 | 2 | 1516 | C |
| 81 | 2 | 1519 | G |
| 81 | 2 | 1521 | G |
| 81 | 2 | 1522 | A |
| 81 | 2 | 1525 | C |
| 81 | 2 | 1532 | G |
| 81 | 2 | 1533 | U |
| 81 | 2 | 1534 | G |
| 81 | 2 | 1535 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1537 | G |
| 81 | 2 | 1540 | G |
| 81 | 2 | 1543 | A |
| 81 | 2 | 1552 | U |
| 81 | 2 | 1553 | A |
| 81 | 2 | 1554 | A |
| 81 | 2 | 1555 | U |
| 81 | 2 | 1556 | U |
| 81 | 2 | 1557 | A |
| 81 | 2 | 1566 | C |
| 81 | 2 | 1569 | C |
| 81 | 2 | 1570 | G |
| 81 | 2 | 1571 | A |
| 81 | 2 | 1580 | U |
| 81 | 2 | 1583 | U |
| 81 | 2 | 1594 | C |
| 81 | 2 | 1595 | A |
| 81 | 2 | 1597 | C |
| 81 | 2 | 1598 | A |
| 81 | 2 | 1599 | G |
| 81 | 2 | 1602 | U |
| 81 | 2 | 1611 | U |
| 81 | 2 | 1614 | G |
| 81 | 2 | 1616 | C |
| 81 | 2 | 1617 | C |
| 81 | 2 | 1623 | C |
| 81 | 2 | 1626 | U |
| 81 | 2 | 1629 | A |
| 81 | 2 | 1630 | C |
| 81 | 2 | 1632 | C |
| 81 | 2 | 1633 | A |
| 81 | 2 | 1635 | C |
| 81 | 2 | 1640 | G |
| 81 | 2 | 1648 | U |
| 81 | 2 | 1654 | U |
| 81 | 2 | 1655 | U |
| 81 | 2 | 1656 | G |
| 81 | 2 | 1667 | U |
| 81 | 2 | 1678 | G |
| 81 | 2 | 1679 | A |
| 81 | 2 | 1680 | U |
| 81 | 2 | 1682 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1685 | U |
| 81 | 2 | 1686 | U |
| 81 | 2 | 1687 | A |
| 81 | 2 | 1688 | G |
| 81 | 2 | 1692 | A |
| 81 | 2 | 1693 | G |
| 81 | 2 | 1694 | G |
| 81 | 2 | 1696 | G |
| 81 | 2 | 1697 | G |
| 81 | 2 | 1698 | C |
| 81 | 2 | 1699 | A |
| 81 | 2 | 1700 | A |
| 81 | 2 | 1701 | C |
| 81 | 2 | 1702 | U |
| 81 | 2 | 1703 | C |
| 81 | 2 | 1706 | U |
| 81 | 2 | 1707 | C |
| 81 | 2 | 1708 | U |
| 81 | 2 | 1709 | C |
| 81 | 2 | 1710 | A |
| 81 | 2 | 1711 | G |
| 81 | 2 | 1712 | A |
| 81 | 2 | 1725 | G |
| 81 | 2 | 1729 | A |
| 81 | 2 | 1733 | U |
| 81 | 2 | 1737 | C |
| 81 | 2 | 1740 | U |
| 81 | 2 | 1743 | G |
| 81 | 2 | 1744 | A |
| 81 | 2 | 1745 | G |
| 81 | 2 | 1748 | A |
| 81 | 2 | 1751 | A |
| 81 | 2 | 1752 | A |
| 81 | 2 | 1753 | A |
| 81 | 2 | 1754 | A |
| 81 | 2 | 1755 | G |
| 81 | 2 | 1758 | G |
| 81 | 2 | 1759 | U |
| 81 | 2 | 1760 | A |
| 81 | 2 | 1763 | A |
| 81 | 2 | 1764 | A |
| 81 | 2 | 1766 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1767 | U |
| 81 | 2 | 1770 | C |
| 81 | 2 | 1777 | U |
| 81 | 2 | 1778 | G |
| 81 | 2 | 1779 | A |
| 81 | 2 | 1780 | A |
| 81 | 2 | 1781 | C |
| 81 | 2 | 1789 | A |
| 81 | 2 | 1790 | G |
| 81 | 2 | 1791 | G |
| 81 | 2 | 1792 | A |
| 81 | 2 | 1793 | U |
| 81 | 2 | 1794 | C |
| 81 | 2 | 1796 | U |
| 81 | 2 | 1798 | A |
| 82 | 4 | 6038 | G |
| 82 | 4 | 6039 | A |
| 82 | 4 | 6042 | U |
| 82 | 4 | 6044 | G |
| 82 | 4 | 6048 | G |
| 82 | 4 | 6054 | A |
| 82 | 4 | 6055 | C |
| 82 | 4 | 6056 | A |
| 82 | 4 | 6059 | U |
| 82 | 4 | 6060 | U |
| 82 | 4 | 6061 | U |
| 82 | 4 | 6067 | G |
| 82 | 4 | 6068 | U |
| 82 | 4 | 6069 | U |
| 82 | 4 | 6071 | A |
| 82 | 4 | 6072 | U |
| 82 | 4 | 6073 | A |
| 82 | 4 | 6074 | A |
| 82 | 4 | 6086 | U |
| 82 | 4 | 6088 | C |
| 82 | 4 | 6089 | U |
| 82 | 4 | 6090 | A |
| 82 | 4 | 6098 | A |
| 82 | 4 | 6101 | U |
| 82 | 4 | 6106 | U |
| 82 | 4 | 6107 | A |
| 82 | 4 | 6108 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 82 | 4 | 6113 | U |
| 82 | 4 | 6116 | G |
| 82 | 4 | 6117 | C |
| 82 | 4 | 6118 | U |
| 82 | 4 | 6119 | U |
| 82 | 4 | 6120 | U |
| 82 | 4 | 6121 | A |
| 82 | 4 | 6122 | C |
| 82 | 4 | 6123 | G |
| 82 | 4 | 6124 | U |
| 82 | 4 | 6125 | U |
| 82 | 4 | 6126 | C |
| 82 | 4 | 6127 | C |
| 82 | 4 | 6128 | A |
| 82 | 4 | 6129 | G |
| 82 | 4 | 6130 | G |
| 82 | 4 | 6133 | G |
| 82 | 4 | 6134 | C |
| 82 | 4 | 6135 | C |
| 82 | 4 | 6137 | A |
| 82 | 4 | 6138 | G |
| 82 | 4 | 6140 | G |
| 82 | 4 | 6142 | C |
| 82 | 4 | 6144 | G |
| 82 | 4 | 6145 | C |
| 82 | 4 | 6146 | C |
| 82 | 4 | 6147 | C |
| 82 | 4 | 6148 | C |
| 82 | 4 | 6153 | U |
| 82 | 4 | 6158 | A |
| 82 | 4 | 6164 | C |
| 82 | 4 | 6165 | C |
| 82 | 4 | 6166 | C |
| 82 | 4 | 6168 | C |
| 82 | 4 | 6170 | C |
| 82 | 4 | 6172 | A |
| 82 | 4 | 6173 | C |
| 82 | 4 | 6175 | G |
| 82 | 4 | 6176 | U |
| 82 | 4 | 6177 | U |
| 82 | 4 | 6179 | U |
| 82 | 4 | 6180 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 82 | 4 | 6181 | C |
| 82 | 4 | 6182 | A |
| 82 | 4 | 6183 | G |
| 82 | 4 | 6189 | G |
| 82 | 4 | 6192 | G |
| 82 | 4 | 6194 | C |
| 82 | 4 | 6195 | G |
| 82 | 4 | 6196 | A |
| 82 | 4 | 6197 | A |
| 82 | 4 | 6199 | A |
| 82 | 4 | 6200 | A |
| 82 | 4 | 6201 | C |
| 82 | 4 | 6202 | C |
| 82 | 4 | 6203 | U |
| 82 | 4 | 6204 | A |
| 82 | 4 | 6211 | U |
| 82 | 4 | 6212 | U |
| 82 | 4 | 6213 | A |
| 82 | 4 | 6217 | G |
| 82 | 4 | 6218 | C |
| 82 | 4 | 6219 | U |

All (359) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 43 | A |
| 1 | 5 | 65 | A |
| 1 | 5 | 66 | A |
| 1 | 5 | 99 | A |
| 1 | 5 | 112 | U |
| 1 | 5 | 119 | U |
| 1 | 5 | 121 | A |
| 1 | 5 | 156 | A |
| 1 | 5 | 166 | C |
| 1 | 5 | 210 | U |
| 1 | 5 | 217 | U |
| 1 | 5 | 238 | A |
| 1 | 5 | 282 | G |
| 1 | 5 | 283 | G |
| 1 | 5 | 297 | G |
| 1 | 5 | 298 | U |
| 1 | 5 | 420 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 436 | A |
| 1 | 5 | 489 | G |
| 1 | 5 | 518 | C |
| 1 | 5 | 529 | U |
| 1 | 5 | 555 | G |
| 1 | 5 | 561 | G |
| 1 | 5 | 562 | A |
| 1 | 5 | 580 | A |
| 1 | 5 | 593 | U |
| 1 | 5 | 596 | U |
| 1 | 5 | 598 | G |
| 1 | 5 | 609 | C |
| 1 | 5 | 707 | A |
| 1 | 5 | 735 | U |
| 1 | 5 | 736 | C |
| 1 | 5 | 737 | U |
| 1 | 5 | 741 | G |
| 1 | 5 | 757 | A |
| 1 | 5 | 787 | A |
| 1 | 5 | 844 | C |
| 1 | 5 | 859 | A |
| 1 | 5 | 860 | U |
| 1 | 5 | 867 | A |
| 1 | 5 | 887 | G |
| 1 | 5 | 908 | G |
| 1 | 5 | 950 | U |
| 1 | 5 | 952 | U |
| 1 | 5 | 964 | G |
| 1 | 5 | 985 | U |
| 1 | 5 | 987 | C |
| 1 | 5 | 998 | A |
| 1 | 5 | 1004 | U |
| 1 | 5 | 1035 | A |
| 1 | 5 | 1052 | U |
| 1 | 5 | 1065 | U |
| 1 | 5 | 1068 | G |
| 1 | 5 | 1115 | U |
| 1 | 5 | 1155 | A |
| 1 | 5 | 1167 | C |
| 1 | 5 | 1179 | U |
| 1 | 5 | 1193 | G |
| 1 | 5 | 1196 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 1209 | C |
| 1 | 5 | 1212 | U |
| 1 | 5 | 1233 | G |
| 1 | 5 | 1255 | C |
| 1 | 5 | 1257 | A |
| 1 | 5 | 1278 | G |
| 1 | 5 | 1300 | U |
| 1 | 5 | 1316 | G |
| 1 | 5 | 1323 | A |
| 1 | 5 | 1326 | A |
| 1 | 5 | 1390 | A |
| 1 | 5 | 1403 | C |
| 1 | 5 | 1421 | G |
| 1 | 5 | 1452 | A |
| 1 | 5 | 1496 | G |
| 1 | 5 | 1525 | U |
| 1 | 5 | 1531 | G |
| 1 | 5 | 1539 | U |
| 1 | 5 | 1549 | A |
| 1 | 5 | 1558 | A |
| 1 | 5 | 1575 | U |
| 1 | 5 | 1576 | U |
| 1 | 5 | 1598 | U |
| 1 | 5 | 1600 | C |
| 1 | 5 | 1610 | U |
| 1 | 5 | 1685 | U |
| 1 | 5 | 1693 | U |
| 1 | 5 | 1719 | A |
| 1 | 5 | 1747 | G |
| 1 | 5 | 1777 | G |
| 1 | 5 | 1785 | A |
| 1 | 5 | 1788 | U |
| 1 | 5 | 1815 | C |
| 1 | 5 | 1816 | A |
| 1 | 5 | 1827 | A |
| 1 | 5 | 1848 | A |
| 1 | 5 | 1922 | G |
| 1 | 5 | 1924 | C |
| 1 | 5 | 1925 | G |
| 1 | 5 | 2032 | U |
| 1 | 5 | 2040 | U |
| 1 | 5 | 2041 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2050 | A |
| 1 | 5 | 2051 | U |
| 1 | 5 | 2052 | G |
| 1 | 5 | 2058 | A |
| 1 | 5 | 2062 | A |
| 1 | 5 | 2070 | C |
| 1 | 5 | 2079 | G |
| 1 | 5 | 2081 | U |
| 1 | 5 | 2107 | A |
| 1 | 5 | 2113 | A |
| 1 | 5 | 2166 | C |
| 1 | 5 | 2173 | C |
| 1 | 5 | 2218 | G |
| 1 | 5 | 2219 | G |
| 1 | 5 | 2228 | A |
| 1 | 5 | 2235 | U |
| 1 | 5 | 2236 | C |
| 1 | 5 | 2237 | U |
| 1 | 5 | 2238 | U |
| 1 | 5 | 2249 | A |
| 1 | 5 | 2250 | A |
| 1 | 5 | 2252 | G |
| 1 | 5 | 2274 | G |
| 1 | 5 | 2276 | G |
| 1 | 5 | 2278 | A |
| 1 | 5 | 2284 | G |
| 1 | 5 | 2285 | G |
| 1 | 5 | 2341 | A |
| 1 | 5 | 2343 | C |
| 1 | 5 | 2346 | G |
| 1 | 5 | 2369 | G |
| 1 | 5 | 2416 | A |
| 1 | 5 | 2417 | G |
| 1 | 5 | 2422 | U |
| 1 | 5 | 2429 | U |
| 1 | 5 | 2437 | A |
| 1 | 5 | 2455 | A |
| 1 | 5 | 2456 | U |
| 1 | 5 | 2468 | U |
| 1 | 5 | 2469 | A |
| 1 | 5 | 2481 | C |
| 1 | 5 | 2482 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 2491 | U |
| 1 | 5 | 2507 | U |
| 1 | 5 | 2518 | G |
| 1 | 5 | 2529 | C |
| 1 | 5 | 2530 | A |
| 1 | 5 | 2539 | U |
| 1 | 5 | 2540 | A |
| 1 | 5 | 2553 | G |
| 1 | 5 | 2561 | A |
| 1 | 5 | 2586 | G |
| 1 | 5 | 2630 | G |
| 1 | 5 | 2645 | G |
| 1 | 5 | 2648 | A |
| 1 | 5 | 2657 | A |
| 1 | 5 | 2696 | G |
| 1 | 5 | 2722 | G |
| 1 | 5 | 2739 | G |
| 1 | 5 | 2740 | U |
| 1 | 5 | 2745 | G |
| 1 | 5 | 2769 | A |
| 1 | 5 | 2785 | A |
| 1 | 5 | 2786 | U |
| 1 | 5 | 2840 | A |
| 1 | 5 | 2854 | U |
| 1 | 5 | 2866 | G |
| 1 | 5 | 2890 | G |
| 1 | 5 | 2918 | G |
| 1 | 5 | 2922 | U |
| 1 | 5 | 2939 | A |
| 1 | 5 | 3023 | U |
| 1 | 5 | 3024 | U |
| 1 | 5 | 3046 | U |
| 1 | 5 | 3061 | C |
| 1 | 5 | 3122 | C |
| 1 | 5 | 3125 | U |
| 1 | 5 | 3135 | A |
| 1 | 5 | 3140 | A |
| 1 | 5 | 3163 | U |
| 1 | 5 | 3164 | U |
| 1 | 5 | 3186 | A |
| 1 | 5 | 3196 | C |
| 1 | 5 | 3207 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 5 | 3214 | G |
| 1 | 5 | 3220 | G |
| 1 | 5 | 3237 | U |
| 1 | 5 | 3242 | A |
| 1 | 5 | 3245 | U |
| 1 | 5 | 3248 | U |
| 1 | 5 | 3257 | A |
| 1 | 5 | 3261 | U |
| 1 | 5 | 3284 | A |
| 1 | 5 | 3285 | U |
| 1 | 5 | 3308 | G |
| 1 | 5 | 3309 | U |
| 1 | 5 | 3325 | U |
| 2 | 7 | 13 | A |
| 2 | 7 | 49 | G |
| 2 | 7 | 76 | A |
| 2 | 7 | 111 | U |
| 3 | 8 | 7 | U |
| 3 | 8 | 8 | C |
| 3 | 8 | 34 | U |
| 3 | 8 | 79 | A |
| 3 | 8 | 81 | U |
| 3 | 8 | 126 | A |
| 81 | 2 | 2 | A |
| 81 | 2 | 3 | U |
| 81 | 2 | 8 | U |
| 81 | 2 | 10 | G |
| 81 | 2 | 11 | A |
| 81 | 2 | 45 | U |
| 81 | 2 | 66 | U |
| 81 | 2 | 72 | A |
| 81 | 2 | 73 | U |
| 81 | 2 | 114 | C |
| 81 | 2 | 129 | U |
| 81 | 2 | 130 | C |
| 81 | 2 | 131 | C |
| 81 | 2 | 133 | U |
| 81 | 2 | 177 | U |
| 81 | 2 | 186 | G |
| 81 | 2 | 209 | A |
| 81 | 2 | 216 | A |
| 81 | 2 | 217 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81 | 2 | 239 | C |
| 81 | 2 | 248 | U |
| 81 | 2 | 258 | U |
| 81 | 2 | 265 | A |
| 81 | 2 | 277 | U |
| 81 | 2 | 279 | U |
| 81 | 2 | 314 | A |
| 81 | 2 | 321 | G |
| 81 | 2 | 336 | G |
| 81 | 2 | 368 | A |
| 81 | 2 | 398 | A |
| 81 | 2 | 399 | A |
| 81 | 2 | 415 | A |
| 81 | 2 | 439 | U |
| 81 | 2 | 451 | A |
| 81 | 2 | 452 | U |
| 81 | 2 | 454 | C |
| 81 | 2 | 473 | A |
| 81 | 2 | 497 | G |
| 81 | 2 | 509 | G |
| 81 | 2 | 542 | C |
| 81 | 2 | 556 | G |
| 81 | 2 | 557 | U |
| 81 | 2 | 563 | G |
| 81 | 2 | 564 | C |
| 81 | 2 | 570 | G |
| 81 | 2 | 576 | G |
| 81 | 2 | 577 | U |
| 81 | 2 | 605 | A |
| 81 | 2 | 621 | A |
| 81 | 2 | 628 | U |
| 81 | 2 | 638 | U |
| 81 | 2 | 695 | U |
| 81 | 2 | 700 | C |
| 81 | 2 | 704 | C |
| 81 | 2 | 708 | C |
| 81 | 2 | 710 | U |
| 81 | 2 | 719 | U |
| 81 | 2 | 721 | U |
| 81 | 2 | 740 | A |
| 81 | 2 | 766 | U |
| 81 | 2 | 779 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 792 | A |
| 81 | 2 | 794 | U |
| 81 | 2 | 809 | G |
| 81 | 2 | 811 | A |
| 81 | 2 | 826 | C |
| 81 | 2 | 828 | A |
| 81 | 2 | 854 | A |
| 81 | 2 | 884 | G |
| 81 | 2 | 885 | U |
| 81 | 2 | 886 | A |
| 81 | 2 | 909 | C |
| 81 | 2 | 912 | G |
| 81 | 2 | 913 | G |
| 81 | 2 | 927 | U |
| 81 | 2 | 929 | A |
| 81 | 2 | 930 | C |
| 81 | 2 | 931 | U |
| 81 | 2 | 963 | U |
| 81 | 2 | 990 | G |
| 81 | 2 | 1002 | A |
| 81 | 2 | 1003 | U |
| 81 | 2 | 1010 | G |
| 81 | 2 | 1027 | C |
| 81 | 2 | 1033 | C |
| 81 | 2 | 1034 | G |
| 81 | 2 | 1044 | C |
| 81 | 2 | 1056 | U |
| 81 | 2 | 1060 | U |
| 81 | 2 | 1080 | A |
| 81 | 2 | 1090 | A |
| 81 | 2 | 1098 | U |
| 81 | 2 | 1107 | G |
| 81 | 2 | 1157 | C |
| 81 | 2 | 1195 | A |
| 81 | 2 | 1243 | A |
| 81 | 2 | 1286 | A |
| 81 | 2 | 1292 | U |
| 81 | 2 | 1320 | A |
| 81 | 2 | 1343 | A |
| 81 | 2 | 1386 | A |
| 81 | 2 | 1412 | U |
| 81 | 2 | 1442 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 81 | 2 | 1455 | C |
| 81 | 2 | 1470 | C |
| 81 | 2 | 1491 | A |
| 81 | 2 | 1501 | A |
| 81 | 2 | 1515 | U |
| 81 | 2 | 1532 | G |
| 81 | 2 | 1534 | G |
| 81 | 2 | 1556 | U |
| 81 | 2 | 1580 | U |
| 81 | 2 | 1598 | A |
| 81 | 2 | 1613 | C |
| 81 | 2 | 1628 | U |
| 81 | 2 | 1631 | A |
| 81 | 2 | 1632 | C |
| 81 | 2 | 1654 | U |
| 81 | 2 | 1655 | U |
| 81 | 2 | 1678 | G |
| 81 | 2 | 1724 | G |
| 81 | 2 | 1752 | A |
| 81 | 2 | 1759 | U |
| 81 | 2 | 1763 | A |
| 81 | 2 | 1765 | G |
| 81 | 2 | 1792 | A |
| 81 | 2 | 1795 | A |
| 82 | 4 | 6038 | G |
| 82 | 4 | 6106 | U |
| 82 | 4 | 6119 | U |
| 82 | 4 | 6120 | U |
| 82 | 4 | 6122 | C |
| 82 | 4 | 6124 | U |
| 82 | 4 | 6127 | C |
| 82 | 4 | 6133 | G |
| 82 | 4 | 6134 | C |
| 82 | 4 | 6137 | A |
| 82 | 4 | 6144 | G |
| 82 | 4 | 6165 | C |
| 82 | 4 | 6172 | A |
| 82 | 4 | 6174 | G |
| 82 | 4 | 6177 | U |
| 82 | 4 | 6181 | C |
| 82 | 4 | 6194 | C |
| 82 | 4 | 6195 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 82 | 4 | 6196 | A |
| 82 | 4 | 6200 | A |
| 82 | 4 | 6201 | C |
| 82 | 4 | 6203 | U |
| 82 | 4 | 6211 | U |
| 82 | 4 | 6218 | C |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 86 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 |
| 86 | GCP | 1 | 902 | 84 | 25,34,34 | 2.92 | 7 (28%) | 28,54,54 | 1.19 | 2 (7%) |
| 87 | 6EM | 1 | 903 | 83 | 7,9,9 | 1.06 | 1 (14%) | 9,13,13 | 2.65 | 3 (33%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 86 | GCP | 1 | 902 | 84 | - | 0/18/38/38 | 0/3/3/3 |
| 87 | 6EM | 1 | 903 | 83 | - | 0/12/12/12 | 0/0/0/0 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 86 | 1 | 902 | GCP | C4-N9 | -11.20 | 1.32 | 1.47 |
| 86 | 1 | 902 | GCP | C8-N9 | -3.89 | 1.35 | 1.46 |
| 86 | 1 | 902 | GCP | PG-O3G | -3.12 | 1.47 | 1.54 |
| 86 | 1 | 902 | GCP | C5-C6 | -2.53 | 1.48 | 1.53 |
| 87 | 1 | 903 | 6EM | C3-C5 | -2.10 | 1.50 | 1.53 |
| 86 | 1 | 902 | GCP | C2-N1 | -2.09 | 1.35 | 1.44 |
| 86 | 1 | 902 | GCP | PG-O2G | 2.94 | 1.61 | 1.54 |
| 86 | 1 | 902 | GCP | PG-O1G | 5.58 | 1.62 | 1.50 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 87 | 1 | 903 | 6EM | O6-C5-C3 | -3.94 | 115.79 | 120.64 |
| 86 | 1 | 902 | GCP | PA-O3A-PB | -3.90 | 119.83 | 132.39 |
| 86 | 1 | 902 | GCP | O2G-PG-C3B | 2.66 | 112.85 | 106.40 |
| 87 | 1 | 903 | 6EM | C9-N4-C3 | 3.79 | 120.13 | 110.51 |
| 87 | 1 | 903 | 6EM | C3-C5-N7 | 5.00 | 122.06 | 115.23 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 86 | 1 | 902 | GCP | 1 | 0 |
| 87 | 1 | 903 | 6EM | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 47 | KK | 2 |
| 1 | 5 | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 5 | 443:G | O3' | 466:G | P | 31.65 |
| 1 | 5 | 1948:C | O3' | 2019:G | P | 17.88 |
| 1 | KK | 23:UNK | C | 28:UNK | N | 3.41 |
| 1 | KK | 52:UNK | C | 54:UNK | N | 3.29 |