



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2017 – 10:01 PM EST

PDB ID : 5J30
Title : Thermus thermophilus 70S termination complex containing E. coli RF1
Authors : Hoffer, E.D.; Dunham, C.M.
Deposited on : 2016-03-30
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

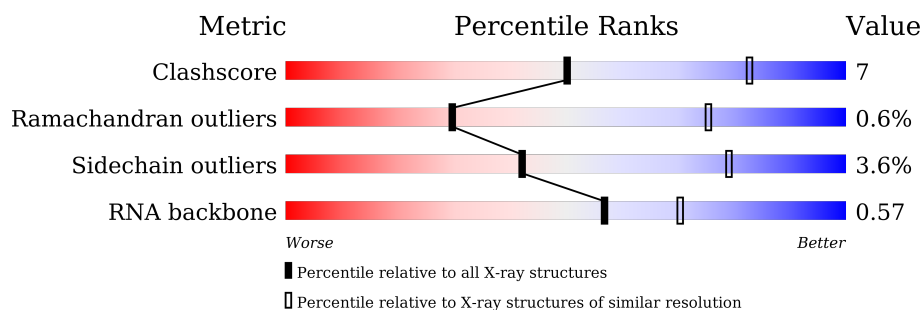
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 1024 (3.22-3.18) |
| Ramachandran outliers | 100387 | 1004 (3.22-3.18) |
| Sidechain outliers | 100360 | 1003 (3.22-3.18) |
| RNA backbone | 2183 | 1079 (3.70-2.70) |


























The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | RA | 2915 | |
| 1 | YA | 2915 | |
| 2 | RB | 122 | |
| 2 | YB | 122 | |
| 3 | RD | 276 | |
| 3 | YD | 276 | |












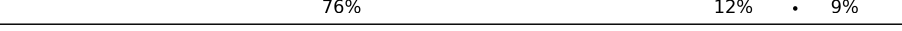







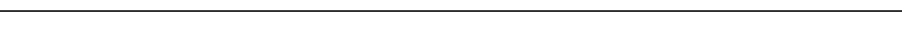

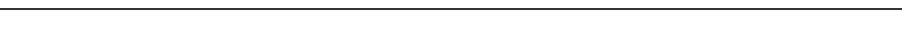
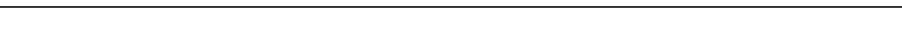


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | RE | 206 |  81% 16% .. |
| 4 | YE | 206 |  78% 19% .. |
| 5 | RF | 210 |  75% 20% .. |
| 5 | YF | 210 |  71% 20% 5% . |
| 6 | RG | 182 |  74% 23% .. |
| 6 | YG | 182 |  63% 32% .. |
| 7 | RH | 180 |  79% 17% .. |
| 7 | YH | 180 |  66% 26% . . |
| 8 | RI | 148 |  78% 20% .. |
| 8 | YI | 148 |  78% 17% .. |
| 9 | RN | 140 |  81% 16% . |
| 9 | YN | 140 |  81% 17% . |
| 10 | RO | 122 |  89% 11% |
| 10 | YO | 122 |  86% 14% |
| 11 | RP | 150 |  79% 19% .. |
| 11 | YP | 150 |  77% 21% .. |
| 12 | RQ | 141 |  79% 20% . |
| 12 | YQ | 141 |  79% 18% . |
| 13 | RR | 118 |  81% 17% . |
| 13 | YR | 118 |  81% 19% |
| 14 | RS | 112 |  85% 12% .. |
| 14 | YS | 112 |  78% 20% .. |
| 15 | RT | 146 |  68% 21% . 10% |
| 15 | YT | 146 |  75% 14% . 10% |
| 16 | RU | 118 |  83% 14% .. |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 16 | YU | 118 |  84% 14% .. |
| 17 | RV | 101 |  89% 10% . |
| 17 | YV | 101 |  75% 22% . |
| 18 | RW | 113 |  82% 13% .. |
| 18 | YW | 113 |  89% 8% .. |
| 19 | RX | 96 |  79% 20% . |
| 19 | YX | 96 |  78% 21% . |
| 20 | RY | 110 |  77% 18% .. |
| 20 | YY | 110 |  72% 24% .. |
| 21 | RZ | 206 |  76% 15% . 8% |
| 21 | YZ | 206 |  73% 17% . 8% |
| 22 | R0 | 85 |  76% 12% . 9% |
| 22 | Y0 | 85 |  72% 19% 9% |
| 23 | R1 | 98 |  84% 13% .. |
| 23 | Y1 | 98 |  74% 20% . .. |
| 24 | R2 | 72 |  88% 8% .. |
| 24 | Y2 | 72 |  81% 15% .. |
| 25 | R3 | 60 |  92% 7% . |
| 25 | Y3 | 60 |  77% 18% .. |
| 26 | R4 | 71 |  56% 37% . .. |
| 26 | Y4 | 71 |  55% 37% 6% . |
| 27 | R5 | 60 |  75% 22% .. |
| 27 | Y5 | 60 |  85% 12% .. |
| 28 | R6 | 54 |  76% 20% .. |
| 28 | Y6 | 54 |  87% 11% . |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 29 | R7 | 49 |  76% 22% . |
| 29 | Y7 | 49 |  78% 20% . |
| 30 | R8 | 65 |  69% 28% .. |
| 30 | Y8 | 65 |  78% 18% .. |
| 31 | R9 | 37 |  81% 19% |
| 31 | Y9 | 37 |  70% 30% |
| 32 | QA | 1521 |  63% 29% 5% .. |
| 32 | XA | 1521 |  63% 30% 6% .. |
| 33 | QB | 256 |  59% 29% . 10% |
| 33 | XB | 256 |  57% 30% . 10% |
| 34 | QC | 239 |  72% 14% 14% |
| 34 | XC | 239 |  66% 20% 14% |
| 35 | QD | 209 |  75% 23% . |
| 35 | XD | 209 |  76% 22% . |
| 36 | QE | 162 |  65% 26% 9% |
| 36 | XE | 162 |  69% 23% 9% |
| 37 | QF | 101 |  80% 19% . |
| 37 | XF | 101 |  83% 16% . |
| 38 | QG | 156 |  80% 19% .. |
| 38 | XG | 156 |  81% 18% .. |
| 39 | QH | 138 |  76% 22% .. |
| 39 | XH | 138 |  82% 16% .. |
| 40 | QI | 128 |  72% 25% .. |
| 40 | XI | 128 |  57% 40% .. |
| 41 | QJ | 105 |  61% 30% . 8% |




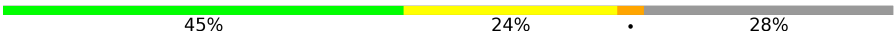
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 41 | XJ | 105 |  |
| 42 | QK | 129 |  |
| 42 | XK | 129 |  |
| 43 | QL | 132 |  |
| 43 | XL | 132 |  |
| 44 | QM | 126 |  |
| 44 | XM | 126 |  |
| 45 | QN | 61 |  |
| 45 | XN | 61 |  |
| 46 | QO | 89 |  |
| 46 | XO | 89 |  |
| 47 | QP | 88 |  |
| 47 | XP | 88 |  |
| 48 | QQ | 105 |  |
| 48 | XQ | 105 |  |
| 49 | QR | 88 |  |
| 49 | XR | 88 |  |
| 50 | QS | 93 |  |
| 50 | XS | 93 |  |
| 51 | QT | 106 |  |
| 51 | XT | 106 |  |
| 52 | QU | 27 |  |
| 52 | XU | 27 |  |
| 53 | QV | 77 |  |
| 53 | XV | 77 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 54 | QX | 25 |  |
| 54 | XX | 25 |  |
| 55 | QY | 360 |  |
| 55 | XY | 360 |  |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294739 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | RA | 2867 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61758 | 27491 | 11552 | 19850 | 2865 | | | |
| 1 | YA | 2867 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61758 | 27491 | 11552 | 19850 | 2865 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | RB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2572 | 1145 | 476 | 832 | 119 | | | |
| 2 | YB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | RD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2131 | 1346 | 422 | 360 | 3 | | | |
| 3 | YD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | RE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |
| 4 | YE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | RF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1584 | 1009 | 298 | 275 | 2 | | | |
| 5 | YF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 297 | 274 | 2 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | RG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1426 | 916 | 253 | 253 | 4 | | | |
| 6 | YG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1424 | 912 | 259 | 249 | 4 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | RH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |
| 7 | YH | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1324 | 842 | 247 | 234 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | RI | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 699 | 191 | 203 | 1 | | | |
| 8 | YI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1076 | 687 | 186 | 202 | 1 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | RN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 722 | 208 | 187 | 4 | | | |
| 9 | YN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | RO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | YO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | RP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |
| 11 | YP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | RQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 12 | YQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | RR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 13 | YR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14 | RS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | |
| 14 | YS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 870 | 549 | 173 | 148 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | RT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 680 | 225 | 185 | 1 | | | |
| 15 | YT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1083 | 675 | 224 | 183 | 1 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | RU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 16 | YU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | RV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 775 | 498 | 141 | 135 | 1 | | | |
| 17 | YV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | RW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |
| 18 | YW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | RX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |
| 19 | YX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | RY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 810 | 520 | 153 | 131 | 6 | | | |
| 20 | YY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 810 | 519 | 153 | 132 | 6 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | RZ | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1485 | 946 | 265 | 272 | 2 | | | |
| 21 | YZ | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1469 | 938 | 259 | 270 | 2 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | R0 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 608 | 375 | 129 | 103 | 1 | | | |
| 22 | Y0 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 608 | 375 | 129 | 103 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | R1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 754 | 475 | 148 | 130 | 1 | | | |
| 23 | Y1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 759 | 478 | 149 | 131 | 1 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | R2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |
| 24 | Y2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 592 | 368 | 119 | 103 | 2 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25 | R3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 25 | Y3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 464 | 296 | 90 | 78 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | R4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 546 | 346 | 96 | 99 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | Y4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 536 | 342 | 98 | 91 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | R5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 27 | Y5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | R6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 28 | Y6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 279 | 91 | 75 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29 | R7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 29 | Y7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30 | R8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 30 | Y8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | R9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 31 | Y9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 32 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 32 | QA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32246 | 14358 | 5975 | 10413 | 1500 | | | |
| 32 | XA | 1504 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32331 | 14396 | 5990 | 10441 | 1504 | | | |

- Molecule 33 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33 | QB | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1842 | 1175 | 330 | 332 | 5 | | | |
| 33 | XB | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1825 | 1167 | 326 | 327 | 5 | | | |

- Molecule 34 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | QC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1558 | 979 | 305 | 273 | 1 | | | |
| 34 | XC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1542 | 968 | 300 | 273 | 1 | | | |

- Molecule 35 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35 | QD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1665 | 1043 | 329 | 286 | 7 | | | |
| 35 | XD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1668 | 1047 | 330 | 284 | 7 | | | |

- Molecule 36 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | QE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 716 | 214 | 199 | 4 | | | |
| 36 | XE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 716 | 214 | 199 | 4 | | | |

- Molecule 37 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | QF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 814 | 516 | 144 | 151 | 3 | | | |
| 37 | XF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 146 | 151 | 3 | | | |

- Molecule 38 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | QG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1235 | 769 | 244 | 216 | 6 | | | |
| 38 | XG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1229 | 766 | 241 | 216 | 6 | | | |

- Molecule 39 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | QH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1098 | 694 | 210 | 192 | 2 | | | |
| 39 | XH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |

- Molecule 40 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40 | QI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 986 | 625 | 193 | 168 | | | |
| 40 | XI | 126 | Total | C | N | O | 0 | 0 | 0 |
| | | | 966 | 613 | 186 | 167 | | | |

- Molecule 41 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41 | QJ | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 719 | 446 | 142 | 131 | | | |
| 41 | XJ | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 710 | 442 | 137 | 131 | | | |

- Molecule 42 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | QK | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 520 | 156 | 155 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | XK | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 833 | 519 | 156 | 155 | 3 | | | |

- Molecule 43 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | QL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 586 | 185 | 159 | 2 | | | |
| 43 | XL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 586 | 185 | 159 | 2 | | | |

- Molecule 44 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | QM | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 914 | 564 | 189 | 159 | 2 | | | |
| 44 | XM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 895 | 550 | 186 | 157 | 2 | | | |

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 45 | QN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 45 | XN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 46 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | QO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 456 | 144 | 126 | 2 | | | |
| 46 | XO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 456 | 144 | 126 | 2 | | | |

- Molecule 47 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | QP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 433 | 134 | 113 | 1 | | | |
| 47 | XP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 677 | 430 | 133 | 113 | 1 | | | |

- Molecule 48 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | QQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |
| 48 | XQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

- Molecule 49 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 49 | QR | 68 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | | |
| 49 | XR | 68 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | | |

- Molecule 50 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | QS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 415 | 120 | 111 | 2 | | | |
| 50 | XS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 645 | 410 | 118 | 115 | 2 | | | |

- Molecule 51 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | QT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 732 | 449 | 157 | 124 | 2 | | | |
| 51 | XT | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 733 | 451 | 154 | 126 | 2 | | | |

- Molecule 52 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 52 | QU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |
| 52 | XU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |

- Molecule 53 is a RNA chain called P-site tRNA fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 53 | QV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 53 | XV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |

- Molecule 54 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 54 | QX | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 215 | 97 | 42 | 66 | 10 | | | |
| 54 | XX | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 193 | 87 | 37 | 60 | 9 | | | |

- Molecule 55 is a protein called Peptide chain release factor 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 55 | QY | 258 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2014 | 1235 | 382 | 389 | 8 | | | |
| 55 | XY | 259 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2023 | 1240 | 384 | 391 | 8 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | QA | 256 | Total | Mg | 0 | 0 |
| | | | 256 | 256 | | |
| 56 | YV | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | RP | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | R7 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | YA | 744 | Total | Mg | 0 | 0 |
| | | | 744 | 744 | | |
| 56 | QM | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | YR | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | RT | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | QD | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | RN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | XE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RG | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | QI | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YD | 9 | Total 9 | Mg 9 | 0 | 0 |
| 56 | XX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QV | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | RX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | YO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | XA | 183 | Total 183 | Mg 183 | 0 | 0 |
| 56 | Y1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RQ | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | R0 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | XT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QL | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RU | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | QG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XJ | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|------------|---------|---------|
| 56 | Y7 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | QH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | YQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | R8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RR | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | RD | 15 | Total 15 | Mg 15 | 0 | 0 |
| 56 | R1 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | XL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YT | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | RV | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | QF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | R5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | Y0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RA | 1039 | Total 1039 | Mg 1039 | 0 | 0 |

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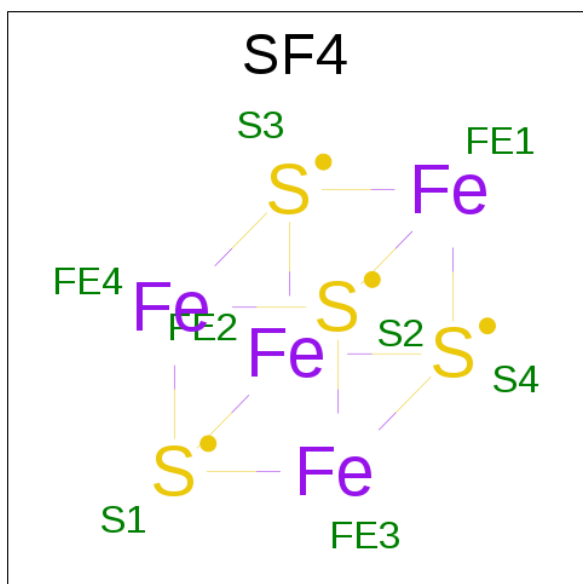
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56 | YF | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | YP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RE | 8 | Total 8 | Mg 8 | 0 | 0 |
| 56 | XK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YB | 18 | Total 18 | Mg 18 | 0 | 0 |
| 56 | XR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QT | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | QN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | YW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | XV | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | RB | 27 | Total 27 | Mg 27 | 0 | 0 |
| 56 | YI | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QE | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | XF | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RF | 12 | Total 12 | Mg 12 | 0 | 0 |
| 56 | R3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | YE | 5 | Total 5 | Mg 5 | 0 | 0 |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57 | Y9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | YY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | Y6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | QN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | XN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | RY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | Y4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | R6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | Y5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | R5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | R4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | R9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

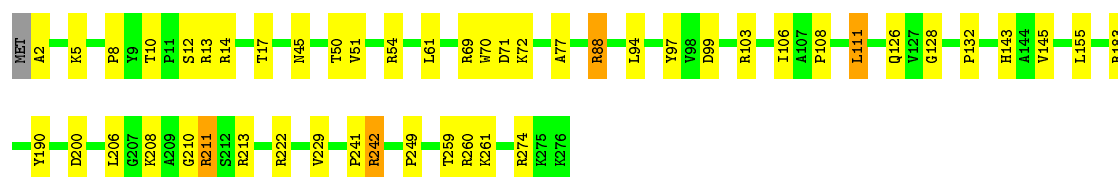
- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 58 | QD | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |
| 58 | XD | 1 | Total 8 | Fe 4 | S 4 | 0 | 0 |

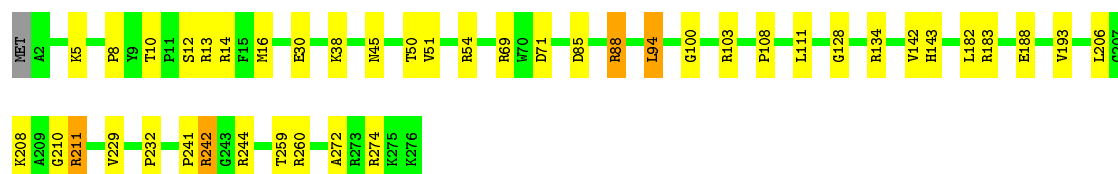
| | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|--------|-------|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1239 | U1240 | A1392 | A1393 | U1503 | A1614 | U1779 | A1927 | A2060 | C2142 | G2238 | C2342 | U2438 | C2573 | U2726 | G2819 |
| G1250 | G1251 | A1396 | U1397 | C1505 | G1622 | A1780 | A1928 | G2061 | C2143 | G2239 | C2343 | A2439 | G2574 | G2732 | G2820 |
| A1253 | A1254 | U1396 | U1397 | C1506 | G1626 | A1784 | G1930 | A2062 | C2144 | U2243 | U2344 | C2440 | G2578 | A2733 | A2821 |
| U1255 | U1256 | U1396 | U1397 | C1507 | G1636 | A1786 | A1932 | G2069 | C2145 | U2244 | A2345 | G2445 | A2602 | A2734 | G2822 |
| G1266 | G1267 | U1396 | U1397 | C1508 | A1637 | U1790 | A1936 | U2074 | G2147 | G2259 | C2347 | A2448 | G2603 | G2735 | A2823 |
| G1270 | G1271 | U1396 | U1397 | C1509 | A1638 | U1791 | A1937 | U2075 | G2148 | U2262 | C2350 | A2449 | G2604 | U2742 | U2832 |
| G1272 | U1273 | U1396 | U1397 | C1509B | A1640 | U1794 | A1938 | U2086 | G2149 | U2263 | G2354 | G2455 | U2609 | C2743 | G2833 |
| A1274 | A1275 | U1396 | U1397 | C1510 | A1641 | U1795 | A1939 | U2087 | G2150 | U2264 | C2355 | G2461 | U2610 | C2744 | U2836 |
| A1278 | U1288 | U1396 | U1397 | C1511 | G1642 | U1796 | U1940 | U2088 | G2151 | A2269 | U2356 | U2462 | U2611 | G2747 | G2838 |
| C1291 | U1292 | U1396 | U1397 | C1512 | G1648 | U1797 | C1941 | U2089 | G2152 | A2274 | G2358 | C2463 | U2612 | A2748 | G2839 |
| C1293 | G1423 | U1396 | U1397 | C1513 | G1653 | U1798 | C1942 | U2090 | G2153 | C2275 | C2359 | C2464 | U2615 | A2749 | U2849 |
| C1297 | G1428 | U1396 | U1397 | C1514 | G1657 | U1799 | C1943 | U2091 | G2154 | C2276 | A2360 | C2465 | C2616 | A2750 | A2850 |
| U1300 | U1301 | U1396 | U1397 | C1515 | G1667 | U1800 | U1955 | U2092 | G2155 | C2277 | C2364 | C2466 | C2617 | C2751 | A2851 |
| U1301 | U1302 | U1396 | U1397 | C1516 | G1668 | U1801 | U1956 | U2093 | G2156 | A2278 | C2365 | C2474 | A2629 | A2752 | G2852 |
| U1313 | C1314 | U1396 | U1397 | C1517 | G1668 | U1802 | U1957 | U2094 | G2157 | C2279 | G2372 | C2475 | G2630 | U2756 | C2853 |
| C1327 | U1352 | U1396 | U1397 | C1518 | G1667 | U1803 | U1958 | U2095 | G2158 | C2280 | G2373 | A2476 | G2643 | U2757 | A2868 |
| G1358 | G1359 | U1396 | U1397 | C1519 | G1667 | U1804 | U1959 | U2096 | G2159 | C2281 | G2374 | A2477 | G2644 | A2758 | G2869 |
| A1360 | A1361 | U1396 | U1397 | C1520 | G1667 | U1805 | U1960 | U2097 | G2160 | C2282 | G2375 | A2478 | G2645 | G2759 | C2870 |
| A1365 | G1368 | U1396 | U1397 | C1521 | G1667 | U1806 | U1961 | U2098 | G2161 | C2283 | G2376 | C2479 | G2646 | A2764 | G2871 |
| G1372 | U1378 | U1396 | U1397 | C1522 | G1667 | U1807 | U1962 | U2099 | G2162 | C2284 | G2377 | C2480 | G2647 | A2765 | G2872 |
| A1378 | A1379 | U1396 | U1397 | C1523 | G1667 | U1808 | U1963 | U2100 | G2163 | C2285 | G2378 | C2481 | G2648 | A2766 | A2873 |
| G1380 | A1494 | U1396 | U1397 | C1524 | G1667 | U1809 | U1964 | U2101 | G2164 | C2286 | G2379 | C2482 | G2649 | C2769 | C2880 |
| A1384 | A1495 | U1396 | U1397 | C1525 | G1667 | U1810 | U1965 | U2102 | G2165 | C2287 | G2380 | C2483 | G2650 | A2778 | A2883 |
| G1385 | A1496 | U1396 | U1397 | C1526 | G1667 | U1811 | U1966 | U2103 | G2166 | C2288 | G2381 | C2484 | G2651 | U2779 | G2886 |
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| | | U1396 | U1397 | C1584 | G1667 | U1869 | U2024 | U2161 | G2224 | C2346 | G2439 | C2542 | G2709 | C | C |
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| | | | | | | | | | | | | | | |
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| A1877 | U1739 | U1739 | A1360 | A1095 | A1095 | A1032 | C923 | C818 | C | | | | | |
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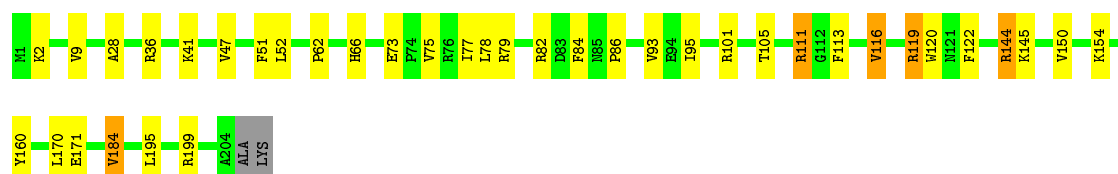
• Molecule 3: 50S ribosomal protein L2

Chain YD: 84% 14% .



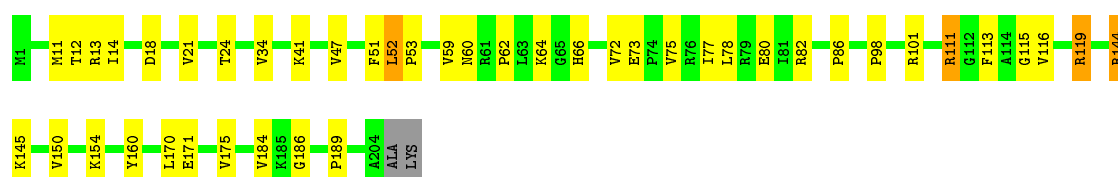
• Molecule 4: 50S ribosomal protein L3

Chain RE: 81% 16% ..



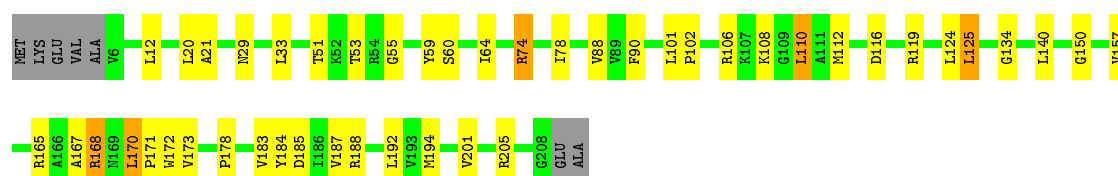
• Molecule 4: 50S ribosomal protein L3

Chain YE: 78% 19% ..



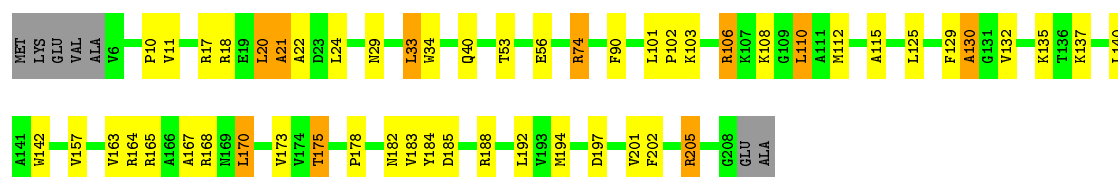
• Molecule 5: 50S ribosomal protein L4

Chain RF: 75% 20% ..



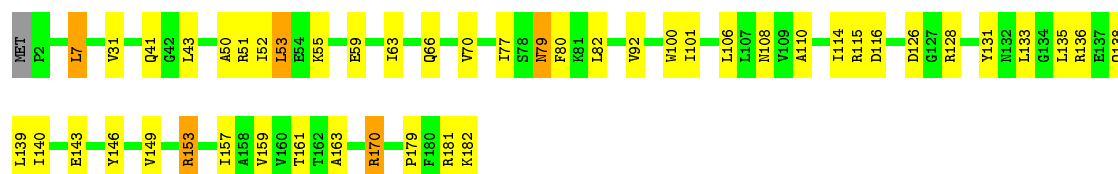
• Molecule 5: 50S ribosomal protein L4

Chain YF: 71% 20% 5% .



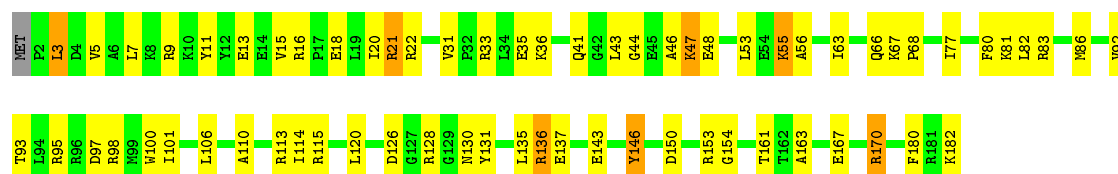
- Molecule 6: 50S ribosomal protein L5

Chain RG: 74% 23% ..



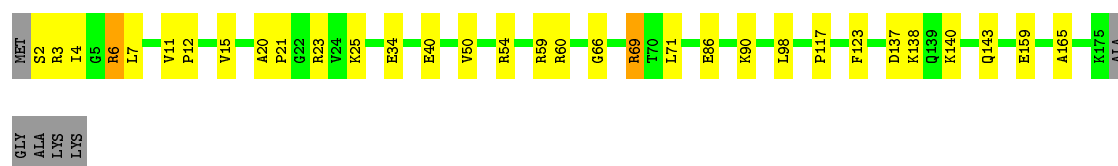
- Molecule 6: 50S ribosomal protein L5

Chain YG: 63% 32% ..



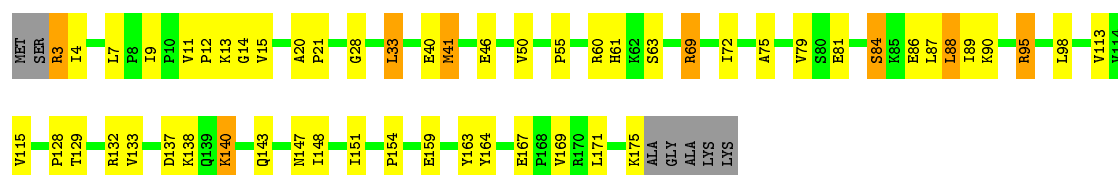
- Molecule 7: 50S ribosomal protein L6

Chain RH: 79% 17% ..



- Molecule 7: 50S ribosomal protein L6

Chain YH: 66% 26% ..



- Molecule 8: 50S ribosomal protein L9

Chain RI: 78% 20% ..



- Molecule 8: 50S ribosomal protein L9

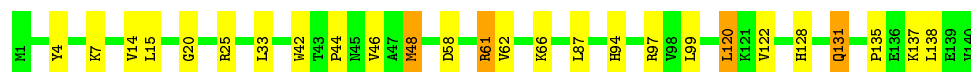
Chain YI: 78% 17%



GLU
GLU

- Molecule 9: 50S ribosomal protein L13

Chain RN: 81% 16%



- Molecule 9: 50S ribosomal protein L13

Chain YN: 81% 17%



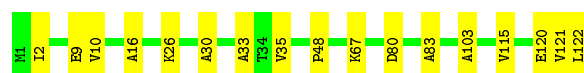
- Molecule 10: 50S ribosomal protein L14

Chain RO: 89% 11%



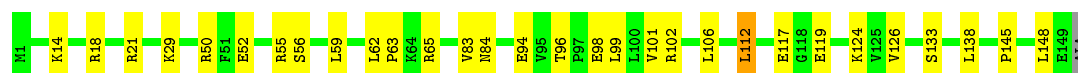
- Molecule 10: 50S ribosomal protein L14

Chain YO: 86% 14%



- Molecule 11: 50S ribosomal protein L15

Chain RP: 79% 19%



- Molecule 11: 50S ribosomal protein L15

Chain YP: 77% 21%



- Molecule 12: 50S ribosomal protein L16

Chain RQ: 79% 20% .



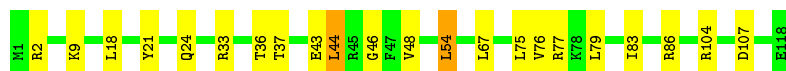
- Molecule 12: 50S ribosomal protein L16

Chain YQ: 79% 18% .



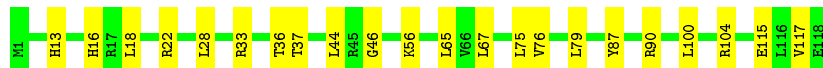
- Molecule 13: 50S ribosomal protein L17

Chain RR: 81% 17% .



- Molecule 13: 50S ribosomal protein L17

Chain YR: 81% 19%



- Molecule 14: 50S ribosomal protein L18

Chain RS: 85% 12% . .



- Molecule 14: 50S ribosomal protein L18

Chain YS: 78% 20% . .




- Molecule 15: 50S ribosomal protein L19

Chain RT: 68% 21% . 10%




GLN
LYS
ALA
GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

- Molecule 15: 50S ribosomal protein L19

Chain YT:  75% 14% 10%




- Molecule 16: 50S ribosomal protein L20

Chain RU:  83% 14% ..



- Molecule 16: 50S ribosomal protein L20

Chain YU:  84% 14% ..




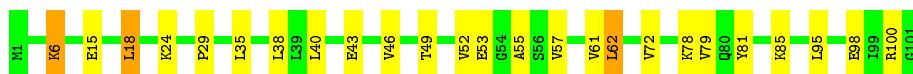
- Molecule 17: 50S ribosomal protein L21

Chain RV:  89% 10% .




- Molecule 17: 50S ribosomal protein L21

Chain YV:  75% 22% .



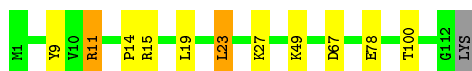
- Molecule 18: 50S ribosomal protein L22

Chain RW:  82% 13% ..




- Molecule 18: 50S ribosomal protein L22

Chain YW:  89% 8% ..




- Molecule 19: 50S ribosomal protein L23

Chain RX:  79% 20%




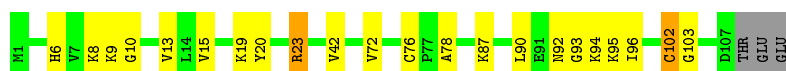
- Molecule 19: 50S ribosomal protein L23

Chain YX:  78% 21%



- Molecule 20: 50S ribosomal protein L24

Chain RY:  77% 18%




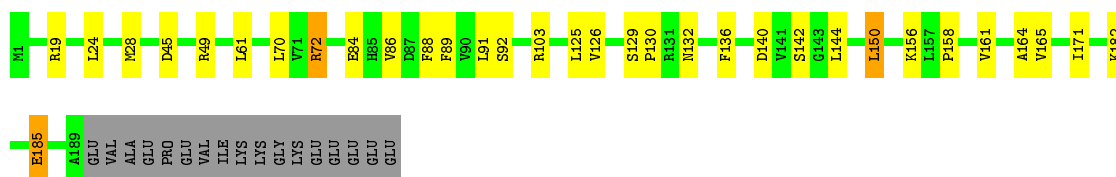
- Molecule 20: 50S ribosomal protein L24

Chain YY:  72% 24%




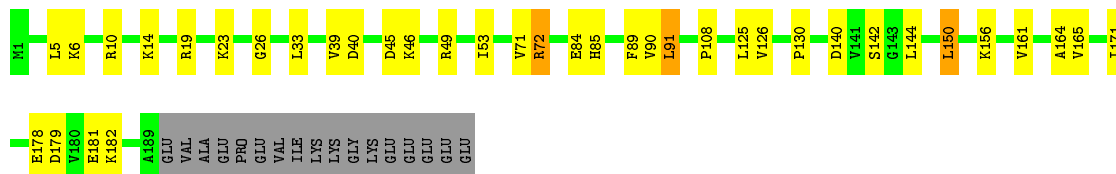
- Molecule 21: 50S ribosomal protein L25

Chain RZ:  76% 15% 8%




- Molecule 21: 50S ribosomal protein L25

Chain YZ:  73% 17% 8%



- Molecule 22: 50S ribosomal protein L27

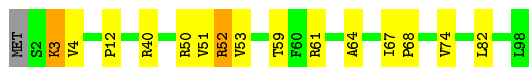
Chain R0:  76% 12% 9%



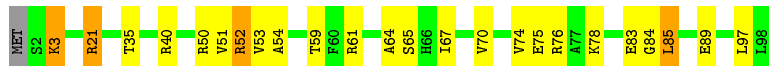
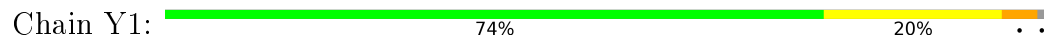
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



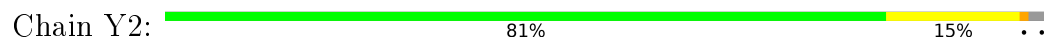
- Molecule 23: 50S ribosomal protein L28



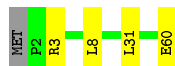
- Molecule 24: 50S ribosomal protein L29



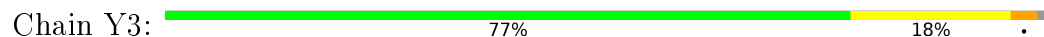
- Molecule 24: 50S ribosomal protein L29



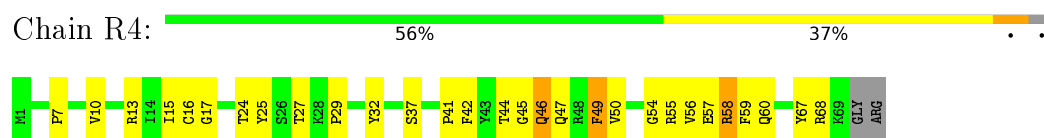
- Molecule 25: 50S ribosomal protein L30



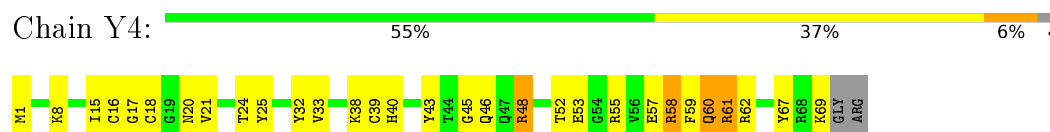
- Molecule 25: 50S ribosomal protein L30



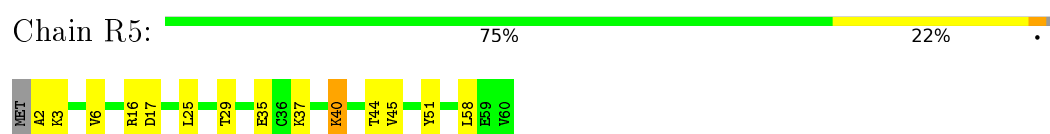
- Molecule 26: 50S ribosomal protein L31



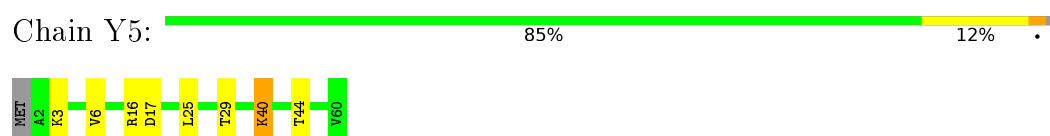
- Molecule 26: 50S ribosomal protein L31



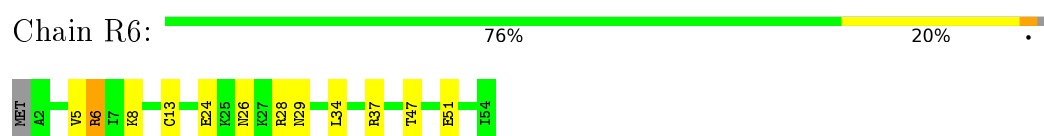
- Molecule 27: 50S ribosomal protein L32



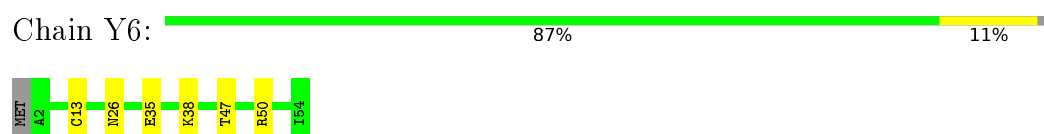
- Molecule 27: 50S ribosomal protein L32



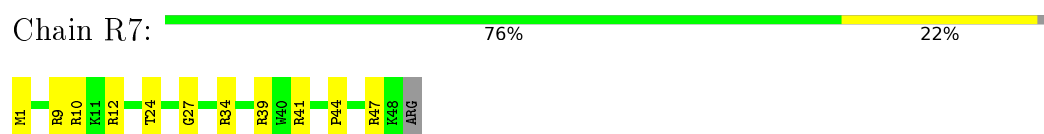
- Molecule 28: 50S ribosomal protein L33



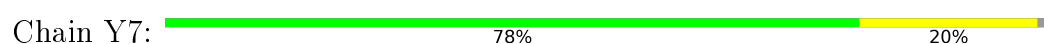
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34





- Molecule 30: 50S ribosomal protein L35

Chain R8: 69% 28% ..



- Molecule 30: 50S ribosomal protein L35

Chain Y8: 78% 18% ..



- Molecule 31: 50S ribosomal protein L36

Chain R9: 81% 19%



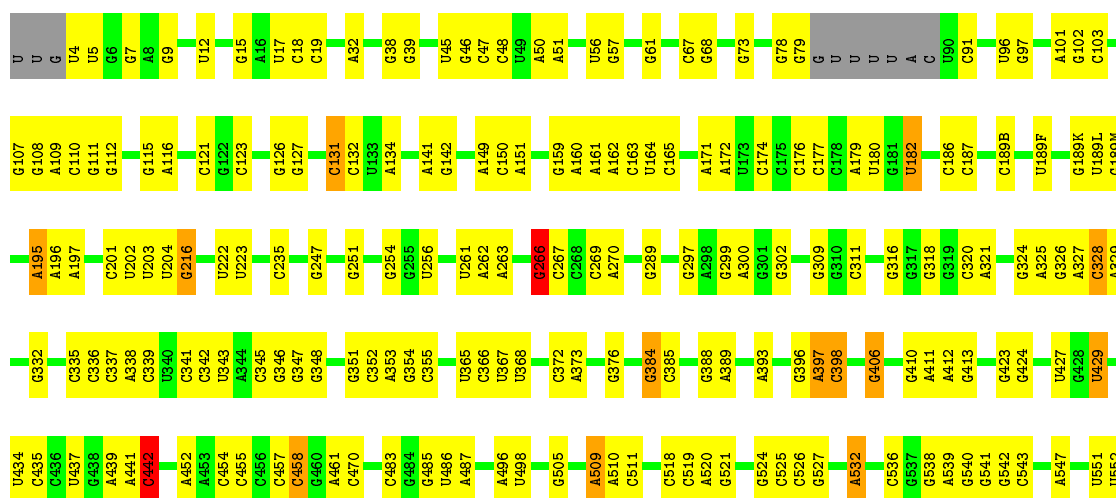
- Molecule 31: 50S ribosomal protein L36

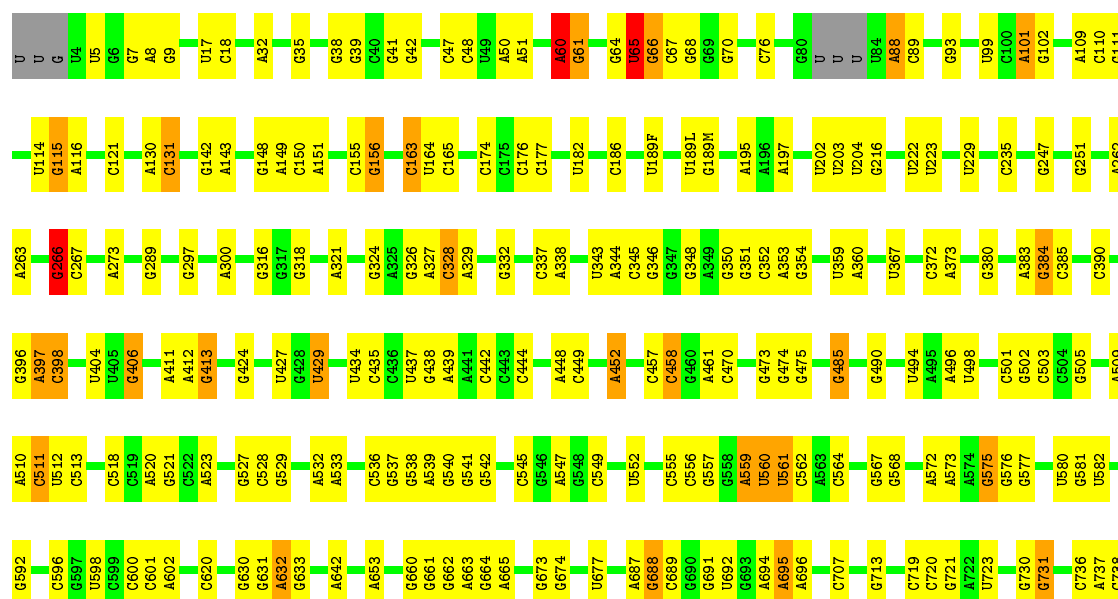
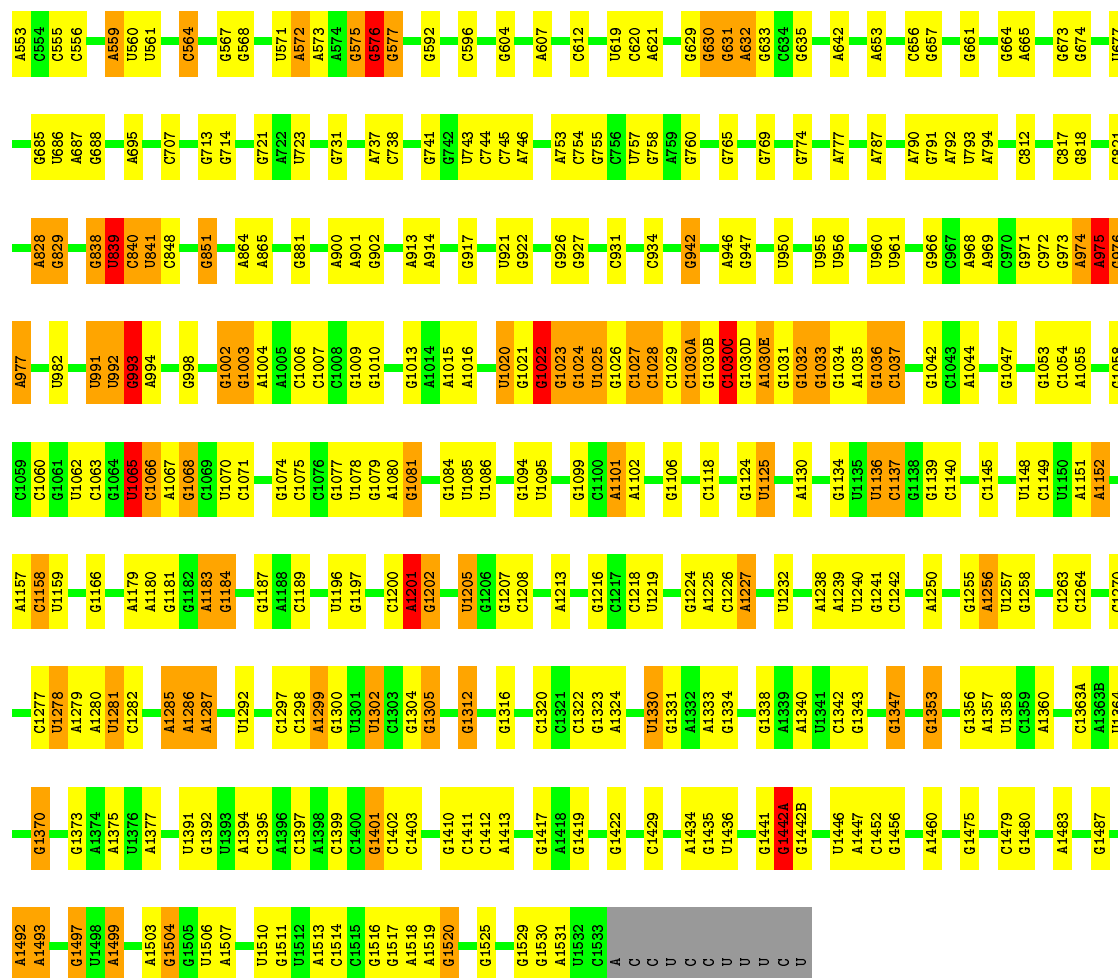
Chain Y9: 70% 30%

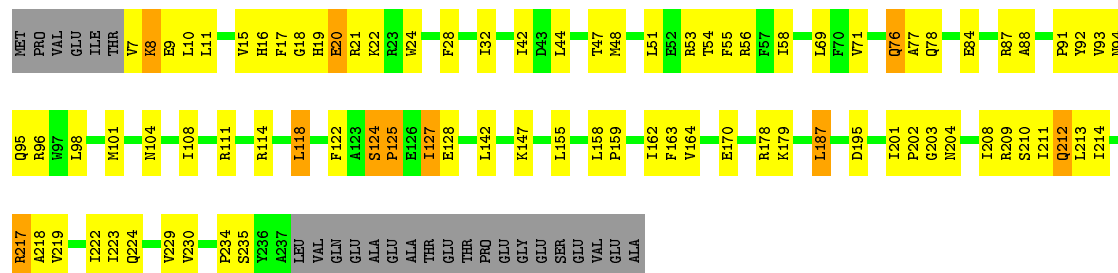


- Molecule 32: 16S rRNA


Chain QA: 63% 29% 5% ..

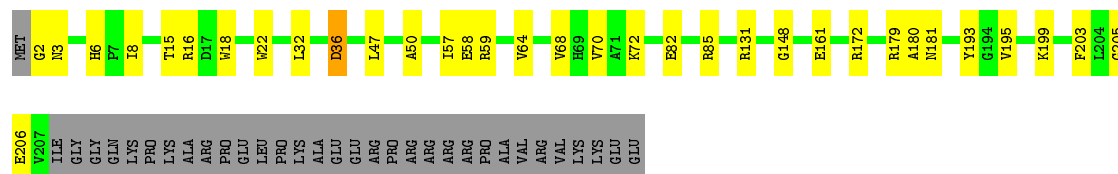






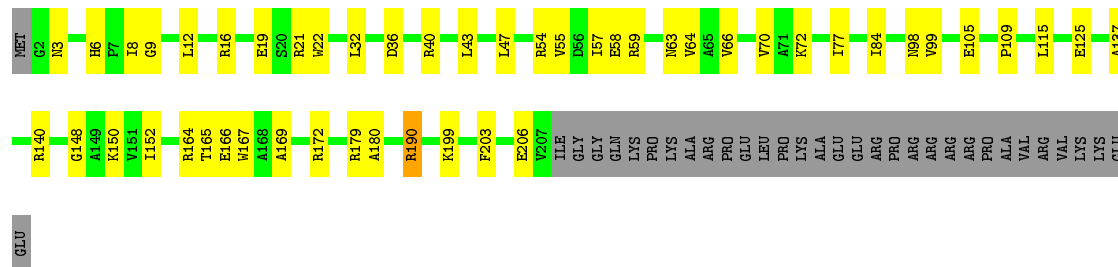
- Molecule 34: 30S ribosomal protein S3

Chain QC:  72% 14% 14%




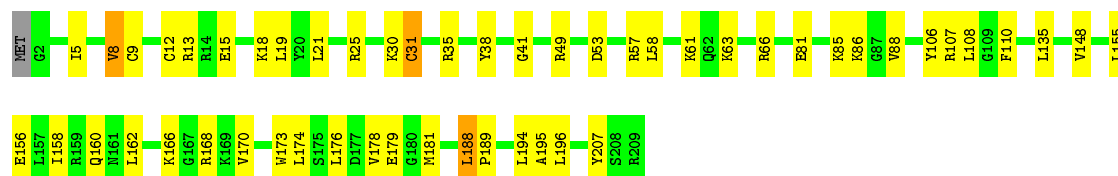
- Molecule 34: 30S ribosomal protein S3

Chain XC:  66% 20% 14%




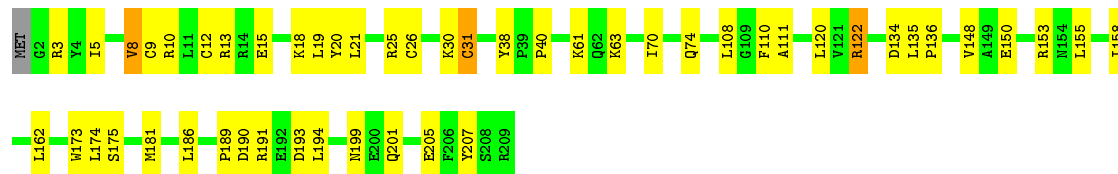
- Molecule 35: 30S ribosomal protein S4

Chain QD:  75% 23% .



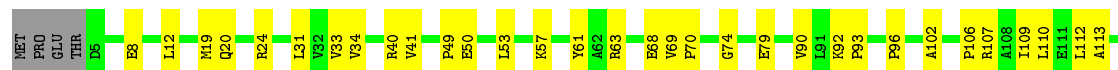
- Molecule 35: 30S ribosomal protein S4

Chain XD:  76% 22% .



- Molecule 36: 30S ribosomal protein S5

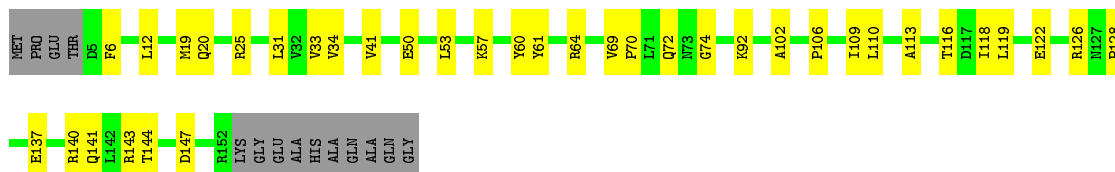
Chain QE:  65% 26% 9%





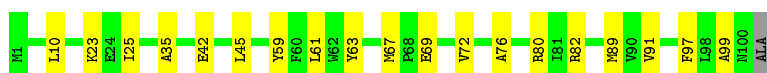
- Molecule 36: 30S ribosomal protein S5

Chain XE: 69% 23% 9%



- Molecule 37: 30S ribosomal protein S6

Chain QF: 80% 19%



- Molecule 37: 30S ribosomal protein S6

Chain XF: 83% 16%



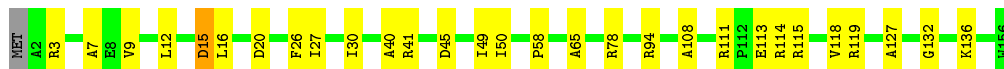
- Molecule 38: 30S ribosomal protein S7

Chain QG: 80% 19%



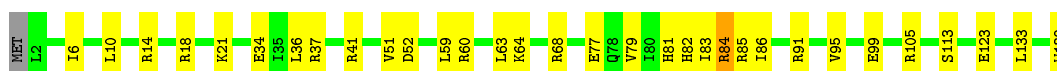
- Molecule 38: 30S ribosomal protein S7

Chain XG: 81% 18%




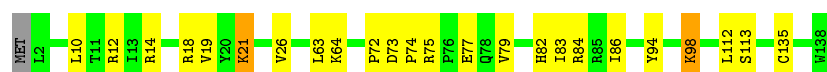
- Molecule 39: 30S ribosomal protein S8

Chain QH: 76% 22%



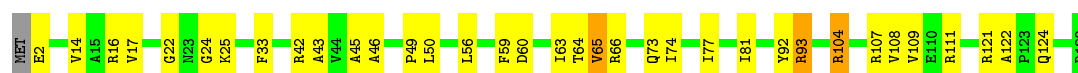
- Molecule 39: 30S ribosomal protein S8

Chain XH:  82% 16% ..



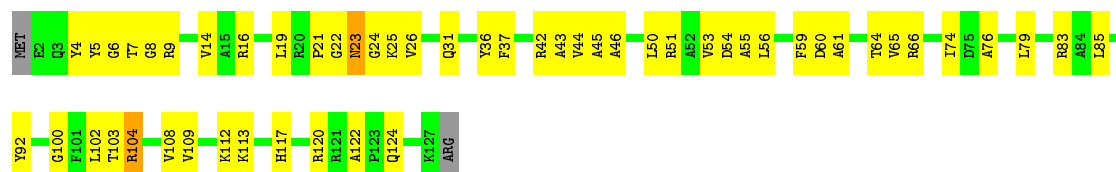
- Molecule 40: 30S ribosomal protein S9

Chain QI:  72% 25% ..



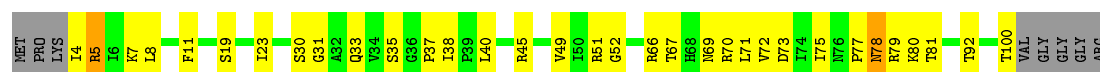
- Molecule 40: 30S ribosomal protein S9

Chain XI:  57% 40% ..



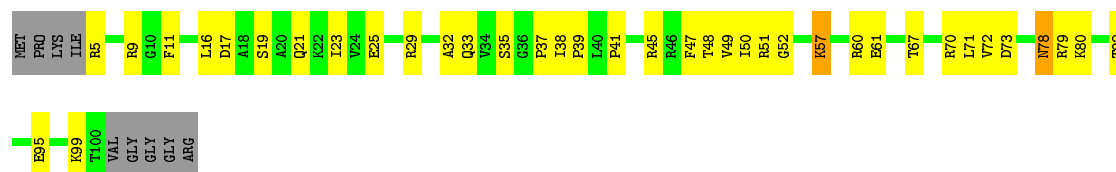
- Molecule 41: 30S ribosomal protein S10

Chain QJ:  61% 30% 8%



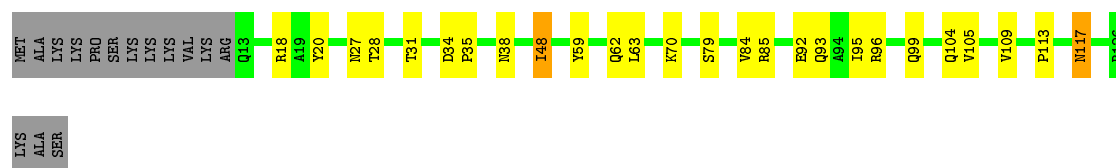
- Molecule 41: 30S ribosomal protein S10

Chain XJ:  55% 34% 9%




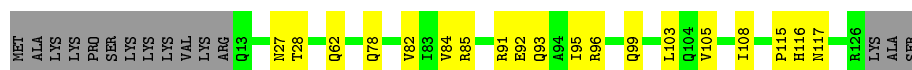
- Molecule 42: 30S ribosomal protein S11

Chain QK:  68% 19% 12%




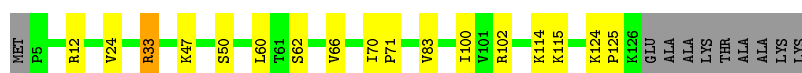
- Molecule 42: 30S ribosomal protein S11

Chain XK:  74% 15% 12%



- Molecule 43: 30S ribosomal protein S12

Chain QL:  80% 12% 8%



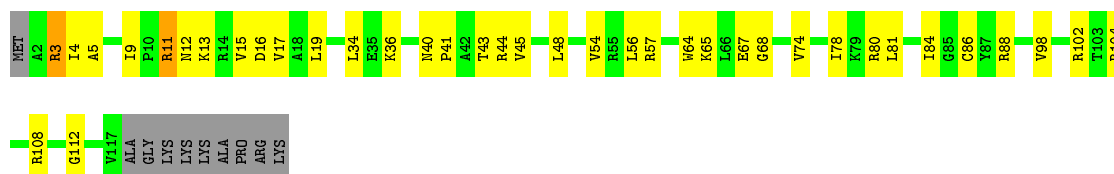
- Molecule 43: 30S ribosomal protein S12

Chain XL:  75% 17% 8%



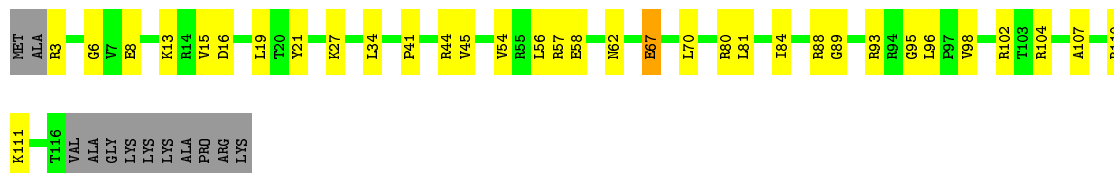
- Molecule 44: 30S ribosomal protein S13

Chain QM:  62% 29% 8%



- Molecule 44: 30S ribosomal protein S13

Chain XM:  63% 26% 10%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain QN:  66% 26% 7%

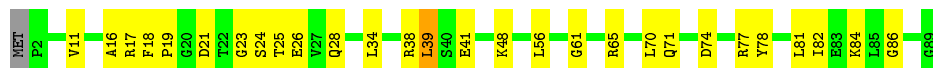


- Molecule 45: 30S ribosomal protein S14 type Z

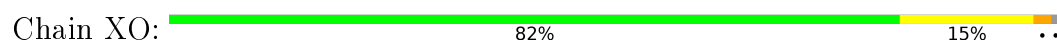
Chain XN:  74% 23% 3%



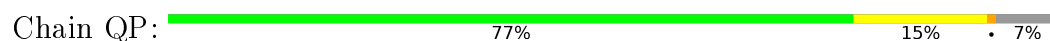
- Molecule 46: 30S ribosomal protein S15



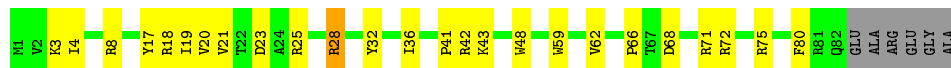
- Molecule 46: 30S ribosomal protein S15



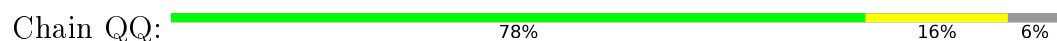
- Molecule 47: 30S ribosomal protein S16



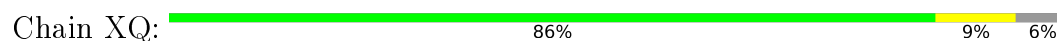
- Molecule 47: 30S ribosomal protein S16



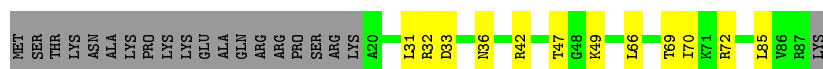
- Molecule 48: 30S ribosomal protein S17



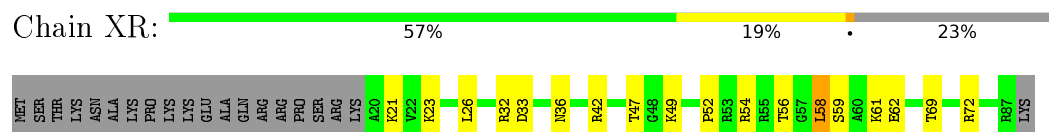
- Molecule 48: 30S ribosomal protein S17



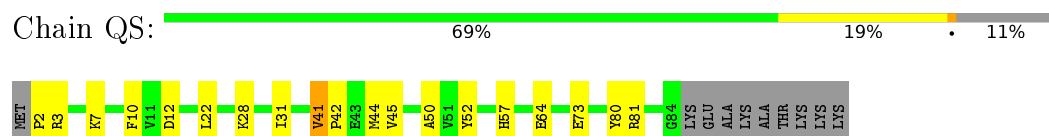
- Molecule 49: 30S ribosomal protein S18



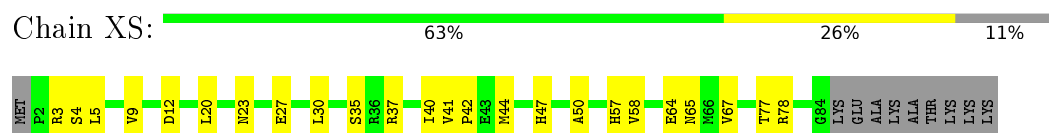
- Molecule 49: 30S ribosomal protein S18



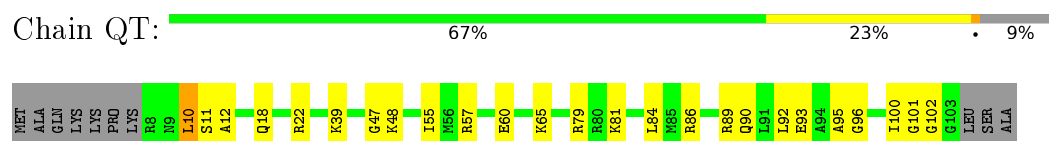
- Molecule 50: 30S ribosomal protein S19



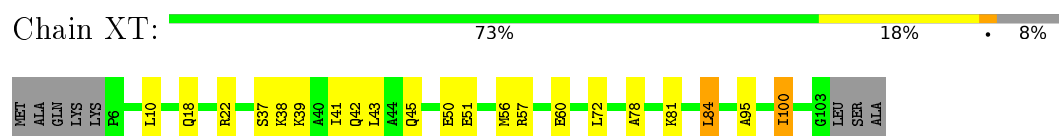
- Molecule 50: 30S ribosomal protein S19



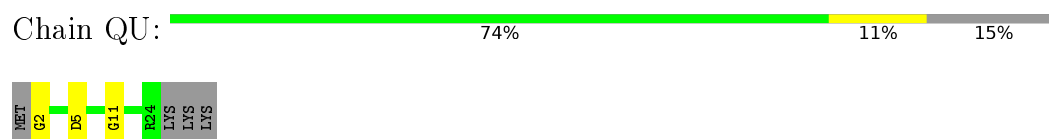
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: P-site tRNA fMet

Chain QV: 



- Molecule 53: P-site tRNA fMet

Chain XV:  62% 29% 9%



- Molecule 54: messenger RNA

Chain QX: 



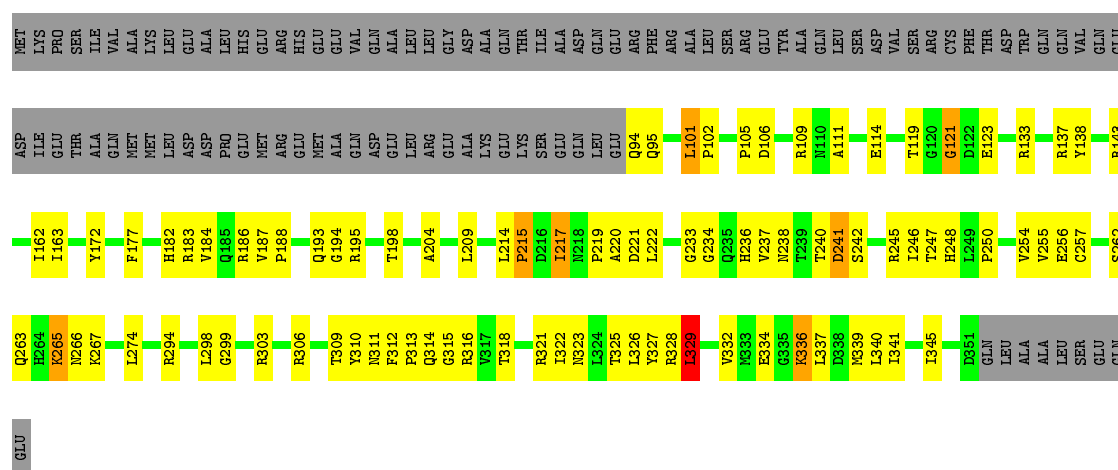
- Molecule 54: messenger RNA

Chain XX: 



- Molecule 55: Peptide chain release factor 1

Chain QY: 



- Molecule 55: Peptide chain release factor 1

Chain XY:  45% 24% 2% 29%





4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.03Å 449.71Å 620.72Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.81 – 3.20 | Depositor |
| % Data completeness (in resolution range) | 99.9 (49.81-3.20) | Depositor |
| R_{merge} | 0.28 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.39 (at 3.19Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.10.1_2155) | Depositor |
| R, R_{free} | 0.214 , 0.244 | Depositor |
| Wilson B-factor (Å ²) | 93.8 | Xtriage |
| Anisotropy | 0.251 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 294739 | wwPDB-VP |
| Average B, all atoms (Å ²) | 117.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MEQ, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | RA | 0.26 | 0/68901 | 0.85 | 52/107544 (0.0%) |
| 1 | YA | 0.30 | 4/68901 (0.0%) | 0.87 | 72/107544 (0.1%) |
| 2 | RB | 0.25 | 0/2876 | 0.83 | 0/4486 |
| 2 | YB | 0.27 | 0/2878 | 0.84 | 0/4490 |
| 3 | RD | 0.30 | 0/2181 | 0.54 | 0/2940 |
| 3 | YD | 0.30 | 0/2186 | 0.56 | 0/2944 |
| 4 | RE | 0.29 | 0/1592 | 0.53 | 0/2149 |
| 4 | YE | 0.31 | 0/1592 | 0.57 | 1/2149 (0.0%) |
| 5 | RF | 0.28 | 0/1619 | 0.52 | 0/2193 |
| 5 | YF | 0.30 | 0/1615 | 0.53 | 0/2188 |
| 6 | RG | 0.28 | 0/1451 | 0.53 | 0/1961 |
| 6 | YG | 0.29 | 0/1449 | 0.52 | 0/1957 |
| 7 | RH | 0.28 | 0/1356 | 0.50 | 0/1834 |
| 7 | YH | 0.29 | 0/1350 | 0.56 | 2/1826 (0.1%) |
| 8 | RI | 0.27 | 0/1109 | 0.54 | 0/1512 |
| 8 | YI | 0.27 | 0/1091 | 0.55 | 1/1490 (0.1%) |
| 9 | RN | 0.28 | 0/1148 | 0.51 | 0/1547 |
| 9 | YN | 0.28 | 0/1144 | 0.50 | 0/1543 |
| 10 | RO | 0.29 | 0/943 | 0.55 | 0/1269 |
| 10 | YO | 0.29 | 0/943 | 0.55 | 0/1269 |
| 11 | RP | 0.28 | 0/1152 | 0.56 | 0/1533 |
| 11 | YP | 0.28 | 0/1152 | 0.56 | 0/1533 |
| 12 | RQ | 0.30 | 0/1143 | 0.52 | 0/1527 |
| 12 | YQ | 0.29 | 0/1143 | 0.51 | 0/1527 |
| 13 | RR | 0.27 | 0/982 | 0.54 | 0/1312 |
| 13 | YR | 0.27 | 0/982 | 0.53 | 0/1312 |
| 14 | RS | 0.27 | 0/887 | 0.52 | 0/1180 |
| 14 | YS | 0.29 | 0/880 | 0.52 | 0/1172 |
| 15 | RT | 0.29 | 0/1105 | 0.58 | 0/1477 |
| 15 | YT | 0.28 | 0/1097 | 0.55 | 0/1468 |
| 16 | RU | 0.29 | 0/977 | 0.45 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | YU | 0.30 | 0/977 | 0.46 | 0/1301 |
| 17 | RV | 0.28 | 0/786 | 0.52 | 0/1053 |
| 17 | YV | 0.32 | 0/782 | 0.57 | 0/1049 |
| 18 | RW | 0.27 | 0/897 | 0.48 | 0/1205 |
| 18 | YW | 0.28 | 0/897 | 0.50 | 0/1205 |
| 19 | RX | 0.30 | 0/764 | 0.53 | 0/1025 |
| 19 | YX | 0.30 | 0/764 | 0.53 | 0/1025 |
| 20 | RY | 0.29 | 0/823 | 0.55 | 0/1099 |
| 20 | YY | 0.33 | 0/823 | 0.55 | 0/1100 |
| 21 | RZ | 0.31 | 0/1517 | 0.53 | 0/2062 |
| 21 | YZ | 0.28 | 0/1501 | 0.52 | 0/2043 |
| 22 | R0 | 0.28 | 0/616 | 0.53 | 0/821 |
| 22 | Y0 | 0.27 | 0/616 | 0.55 | 0/821 |
| 23 | R1 | 0.27 | 0/761 | 0.53 | 0/1013 |
| 23 | Y1 | 0.28 | 0/766 | 0.56 | 0/1018 |
| 24 | R2 | 0.29 | 0/590 | 0.51 | 0/781 |
| 24 | Y2 | 0.26 | 0/594 | 0.46 | 0/785 |
| 25 | R3 | 0.28 | 0/474 | 0.51 | 0/635 |
| 25 | Y3 | 0.29 | 0/469 | 0.54 | 0/630 |
| 26 | R4 | 0.32 | 0/559 | 0.66 | 0/754 |
| 26 | Y4 | 0.37 | 0/549 | 0.63 | 0/741 |
| 27 | R5 | 0.33 | 0/473 | 0.54 | 0/639 |
| 27 | Y5 | 0.32 | 0/469 | 0.54 | 0/635 |
| 28 | R6 | 0.28 | 0/460 | 0.53 | 0/613 |
| 28 | Y6 | 0.23 | 0/456 | 0.46 | 0/608 |
| 29 | R7 | 0.26 | 0/426 | 0.49 | 0/561 |
| 29 | Y7 | 0.26 | 0/426 | 0.45 | 0/561 |
| 30 | R8 | 0.29 | 0/525 | 0.52 | 0/691 |
| 30 | Y8 | 0.28 | 0/525 | 0.51 | 0/691 |
| 31 | R9 | 0.23 | 0/310 | 0.47 | 0/407 |
| 31 | Y9 | 0.26 | 0/310 | 0.51 | 0/407 |
| 32 | QA | 0.26 | 0/35795 | 0.86 | 38/55864 (0.1%) |
| 32 | XA | 0.26 | 0/35890 | 0.85 | 30/56012 (0.1%) |
| 33 | QB | 0.28 | 0/1876 | 0.54 | 0/2533 |
| 33 | XB | 0.30 | 0/1860 | 0.57 | 0/2518 |
| 34 | QC | 0.27 | 0/1582 | 0.52 | 0/2137 |
| 34 | XC | 0.28 | 0/1566 | 0.52 | 0/2119 |
| 35 | QD | 0.28 | 0/1695 | 0.50 | 0/2274 |
| 35 | XD | 0.27 | 0/1698 | 0.47 | 0/2277 |
| 36 | QE | 0.30 | 0/1149 | 0.52 | 0/1548 |
| 36 | XE | 0.28 | 0/1149 | 0.51 | 0/1548 |
| 37 | QF | 0.26 | 0/827 | 0.51 | 0/1120 |
| 37 | XF | 0.26 | 0/829 | 0.52 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | QG | 0.27 | 0/1254 | 0.43 | 0/1683 |
| 38 | XG | 0.27 | 0/1248 | 0.45 | 0/1676 |
| 39 | QH | 0.27 | 0/1118 | 0.50 | 0/1506 |
| 39 | XH | 0.28 | 0/1108 | 0.51 | 0/1494 |
| 40 | QI | 0.28 | 0/1005 | 0.53 | 0/1351 |
| 40 | XI | 0.28 | 0/985 | 0.52 | 0/1329 |
| 41 | QJ | 0.26 | 0/732 | 0.51 | 0/993 |
| 41 | XJ | 0.26 | 0/723 | 0.51 | 0/984 |
| 42 | QK | 0.26 | 0/849 | 0.48 | 0/1150 |
| 42 | XK | 0.26 | 0/848 | 0.53 | 0/1149 |
| 43 | QL | 0.28 | 0/937 | 0.54 | 0/1260 |
| 43 | XL | 0.29 | 0/937 | 0.59 | 0/1260 |
| 44 | QM | 0.26 | 0/924 | 0.52 | 0/1242 |
| 44 | XM | 0.26 | 0/905 | 0.50 | 0/1217 |
| 45 | QN | 0.28 | 0/501 | 0.44 | 0/664 |
| 45 | XN | 0.29 | 0/501 | 0.46 | 0/664 |
| 46 | QO | 0.26 | 0/739 | 0.48 | 0/985 |
| 46 | XO | 0.26 | 0/739 | 0.49 | 0/985 |
| 47 | QP | 0.28 | 0/697 | 0.51 | 0/939 |
| 47 | XP | 0.28 | 0/693 | 0.50 | 0/935 |
| 48 | QQ | 0.26 | 0/836 | 0.50 | 0/1117 |
| 48 | XQ | 0.26 | 0/836 | 0.50 | 0/1117 |
| 49 | QR | 0.26 | 0/560 | 0.51 | 0/746 |
| 49 | XR | 0.26 | 0/560 | 0.51 | 0/746 |
| 50 | QS | 0.27 | 0/663 | 0.57 | 0/895 |
| 50 | XS | 0.27 | 0/660 | 0.55 | 0/893 |
| 51 | QT | 0.27 | 0/734 | 0.48 | 0/969 |
| 51 | XT | 0.27 | 0/736 | 0.42 | 0/976 |
| 52 | QU | 0.25 | 0/203 | 0.52 | 0/266 |
| 52 | XU | 0.30 | 0/203 | 0.52 | 0/266 |
| 53 | QV | 0.33 | 1/1836 (0.1%) | 0.82 | 0/2859 |
| 53 | XV | 0.34 | 1/1836 (0.1%) | 0.82 | 0/2859 |
| 54 | QX | 0.33 | 0/241 | 0.95 | 0/373 |
| 54 | XX | 0.27 | 0/216 | 0.89 | 0/334 |
| 55 | QY | 0.31 | 0/2035 | 0.51 | 0/2742 |
| 55 | XY | 0.29 | 0/2044 | 0.51 | 0/2754 |
| All | All | 0.28 | 6/316288 (0.0%) | 0.78 | 196/472607 (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 |
|-----|-------|---------------------|---------------------|
| 14 | RS | 0 | 1 |
| 26 | R4 | 0 | 1 |
| 33 | QB | 0 | 1 |
| 43 | XL | 0 | 1 |
| All | All | 0 | 4 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 53 | XV | 1 | C | OP3-P | -10.46 | 1.48 | 1.61 |
| 53 | QV | 1 | C | OP3-P | -10.44 | 1.48 | 1.61 |
| 1 | YA | 2751 | G | N1-C2 | -8.70 | 1.30 | 1.37 |
| 1 | YA | 2751 | G | C2-N3 | -6.96 | 1.27 | 1.32 |
| 1 | YA | 1029 | A | N3-C4 | -5.78 | 1.31 | 1.34 |
| 1 | YA | 1050 | A | C2-N3 | -5.73 | 1.28 | 1.33 |

All (196) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | YA | 1029 | A | N1-C2-N3 | 12.53 | 135.56 | 129.30 |
| 32 | QA | 576 | G | OP1-P-O3' | -11.19 | 80.59 | 105.20 |
| 1 | RA | 2602 | A | OP2-P-O3' | -11.18 | 80.60 | 105.20 |
| 32 | QA | 576 | G | OP2-P-O3' | -10.40 | 82.31 | 105.20 |
| 1 | RA | 1050 | A | N1-C2-N3 | 10.32 | 134.46 | 129.30 |
| 1 | YA | 277 | C | C5-C4-N4 | -10.13 | 113.11 | 120.20 |
| 1 | YA | 2187 | G | C5-C6-O6 | -9.72 | 122.77 | 128.60 |
| 1 | RA | 2187 | G | C5-C6-O6 | -9.53 | 122.88 | 128.60 |
| 1 | RA | 1050 | A | C2-N3-C4 | -9.28 | 105.96 | 110.60 |
| 32 | XA | 1158 | C | C2-N1-C1' | 8.99 | 128.69 | 118.80 |
| 1 | YA | 277 | C | C6-N1-C1' | -8.50 | 110.60 | 120.80 |
| 1 | YA | 1050 | A | C5-N7-C8 | -8.46 | 99.67 | 103.90 |
| 1 | RA | 1050 | A | C5-C6-N1 | -8.28 | 113.56 | 117.70 |
| 1 | YA | 1050 | A | N7-C8-N9 | 8.24 | 117.92 | 113.80 |
| 1 | YA | 2751 | G | C2-N3-C4 | 8.14 | 115.97 | 111.90 |
| 1 | RA | 1050 | A | C4-C5-C6 | 8.10 | 121.05 | 117.00 |
| 1 | YA | 1029 | A | C6-N1-C2 | -8.05 | 113.77 | 118.60 |
| 1 | YA | 2465 | C | N1-C2-O2 | 7.72 | 123.53 | 118.90 |
| 1 | RA | 1092 | C | N1-C2-O2 | 7.72 | 123.53 | 118.90 |
| 32 | XA | 1158 | C | N1-C2-O2 | 7.70 | 123.52 | 118.90 |
| 1 | YA | 2187 | G | N1-C6-O6 | 7.68 | 124.51 | 119.90 |
| 32 | QA | 1036 | G | C5-C6-O6 | -7.61 | 124.03 | 128.60 |
| 1 | RA | 2187 | G | N1-C6-O6 | 7.60 | 124.46 | 119.90 |
| 1 | YA | 1092 | C | N1-C2-O2 | 7.53 | 123.42 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | YA | 2187 | G | C6-C5-N7 | -7.43 | 125.94 | 130.40 |
| 32 | QA | 1030(C) | C | C2-N1-C1' | 7.36 | 126.90 | 118.80 |
| 1 | RA | 1097 | U | C2-N1-C1' | 7.34 | 126.51 | 117.70 |
| 32 | QA | 1030(C) | C | N1-C2-O2 | 7.28 | 123.27 | 118.90 |
| 1 | YA | 2187 | G | C4-C5-N7 | 7.26 | 113.70 | 110.80 |
| 32 | QA | 577 | G | OP1-P-OP2 | 7.24 | 130.47 | 119.60 |
| 1 | YA | 2742 | C | O5'-P-OP1 | -7.13 | 99.28 | 105.70 |
| 1 | YA | 277 | C | C2-N1-C1' | 7.07 | 126.57 | 118.80 |
| 32 | XA | 1158 | C | C6-N1-C2 | -7.03 | 117.49 | 120.30 |
| 1 | RA | 2603 | G | OP1-P-OP2 | 7.00 | 130.10 | 119.60 |
| 32 | QA | 1022 | G | C5-C6-O6 | -6.99 | 124.41 | 128.60 |
| 1 | RA | 1092 | C | C2-N1-C1' | 6.99 | 126.48 | 118.80 |
| 1 | RA | 2602 | A | OP1-P-O3' | -6.94 | 89.93 | 105.20 |
| 1 | RA | 2102 | U | N1-C2-O2 | -6.86 | 118.00 | 122.80 |
| 1 | YA | 1092 | C | C2-N1-C1' | 6.85 | 126.33 | 118.80 |
| 32 | XA | 1003 | G | C4-N9-C1' | 6.85 | 135.40 | 126.50 |
| 1 | YA | 1028 | A | N9-C4-C5 | -6.83 | 103.07 | 105.80 |
| 32 | XA | 266 | G | P-O3'-C3' | 6.82 | 127.89 | 119.70 |
| 1 | YA | 277 | C | N3-C4-N4 | 6.78 | 122.74 | 118.00 |
| 32 | XA | 754 | C | N1-C2-O2 | 6.75 | 122.95 | 118.90 |
| 1 | YA | 2102 | U | N1-C2-O2 | -6.74 | 118.08 | 122.80 |
| 1 | YA | 1097 | U | C2-N1-C1' | 6.72 | 125.77 | 117.70 |
| 1 | YA | 2187 | G | N3-C4-N9 | 6.71 | 130.03 | 126.00 |
| 1 | YA | 512 | G | O4'-C1'-N9 | 6.62 | 113.50 | 108.20 |
| 1 | YA | 1029 | A | C2-N3-C4 | -6.61 | 107.30 | 110.60 |
| 32 | QA | 1036 | G | C4-C5-N7 | 6.59 | 113.44 | 110.80 |
| 1 | YA | 1030 | G | N1-C6-O6 | 6.58 | 123.85 | 119.90 |
| 32 | XA | 1183 | A | P-O3'-C3' | 6.57 | 127.58 | 119.70 |
| 1 | YA | 2573 | C | N3-C4-C5 | 6.57 | 124.53 | 121.90 |
| 1 | RA | 2104 | G | N3-C4-N9 | 6.55 | 129.93 | 126.00 |
| 32 | XA | 1054 | C | N1-C2-O2 | 6.54 | 122.83 | 118.90 |
| 32 | QA | 1322 | C | N1-C2-O2 | -6.53 | 114.98 | 118.90 |
| 1 | YA | 1030 | G | C4-C5-N7 | 6.51 | 113.41 | 110.80 |
| 1 | YA | 1125 | G | N3-C4-C5 | -6.45 | 125.37 | 128.60 |
| 32 | XA | 1158 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 8 | YI | 75 | LEU | CA-CB-CG | 6.41 | 130.04 | 115.30 |
| 1 | YA | 1097 | U | N3-C2-O2 | -6.40 | 117.72 | 122.20 |
| 1 | YA | 1028 | A | N3-C4-N9 | 6.35 | 132.48 | 127.40 |
| 32 | QA | 1030(C) | C | N3-C2-O2 | -6.35 | 117.46 | 121.90 |
| 32 | XA | 754 | C | C2-N1-C1' | 6.35 | 125.78 | 118.80 |
| 1 | YA | 2104 | G | N3-C4-N9 | 6.34 | 129.81 | 126.00 |
| 1 | RA | 2187 | G | C4-C5-N7 | 6.34 | 113.33 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | YA | 1313 | U | C2-N1-C1' | 6.32 | 125.29 | 117.70 |
| 1 | YA | 1028 | A | C5-C6-N1 | 6.29 | 120.84 | 117.70 |
| 1 | YA | 1097 | U | N1-C2-O2 | 6.29 | 127.20 | 122.80 |
| 1 | YA | 1125 | G | N3-C4-N9 | 6.27 | 129.76 | 126.00 |
| 1 | YA | 1092 | C | C5-C6-N1 | 6.27 | 124.13 | 121.00 |
| 1 | RA | 2187 | G | C6-C5-N7 | -6.25 | 126.65 | 130.40 |
| 32 | XA | 1003 | G | N7-C8-N9 | 6.23 | 116.21 | 113.10 |
| 1 | YA | 2187 | G | N9-C4-C5 | -6.19 | 102.93 | 105.40 |
| 1 | RA | 2573 | C | N3-C4-C5 | 6.18 | 124.37 | 121.90 |
| 1 | RA | 1097 | U | N3-C2-O2 | -6.18 | 117.88 | 122.20 |
| 1 | RA | 1092 | C | C5-C6-N1 | 6.17 | 124.08 | 121.00 |
| 32 | QA | 1036 | G | N3-C4-N9 | 6.16 | 129.70 | 126.00 |
| 32 | XA | 1003 | G | N3-C4-C5 | -6.16 | 125.52 | 128.60 |
| 1 | RA | 1097 | U | N1-C2-O2 | 6.15 | 127.11 | 122.80 |
| 1 | YA | 1030 | G | C6-C5-N7 | -6.14 | 126.72 | 130.40 |
| 1 | RA | 1082 | U | C2-N1-C1' | 6.09 | 125.00 | 117.70 |
| 1 | RA | 512 | G | O4'-C1'-N9 | 6.07 | 113.05 | 108.20 |
| 32 | XA | 88 | A | C5-C6-N6 | -6.03 | 118.88 | 123.70 |
| 32 | XA | 1003 | G | C8-N9-C4 | -6.01 | 104.00 | 106.40 |
| 1 | RA | 1092 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 32 | QA | 1322 | C | N1-C2-N3 | 5.96 | 123.37 | 119.20 |
| 32 | XA | 1158 | C | C6-N1-C1' | -5.95 | 113.66 | 120.80 |
| 1 | RA | 1092 | C | N3-C2-O2 | -5.95 | 117.74 | 121.90 |
| 1 | YA | 226 | G | O4'-C1'-N9 | 5.93 | 112.94 | 108.20 |
| 1 | YA | 1082 | U | C2-N1-C1' | 5.90 | 124.78 | 117.70 |
| 32 | QA | 754 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 32 | QA | 1030(C) | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 1 | YA | 847 | U | N1-C2-O2 | 5.87 | 126.91 | 122.80 |
| 32 | XA | 65 | U | P-O3'-C3' | 5.85 | 126.72 | 119.70 |
| 32 | XA | 88 | A | N1-C6-N6 | 5.83 | 122.10 | 118.60 |
| 1 | YA | 1092 | C | C6-N1-C2 | -5.81 | 117.98 | 120.30 |
| 32 | XA | 1004 | A | O4'-C1'-N9 | 5.77 | 112.81 | 108.20 |
| 32 | QA | 1285 | A | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 1 | YA | 1092 | C | N3-C2-O2 | -5.75 | 117.87 | 121.90 |
| 1 | YA | 1372 | U | N1-C2-O2 | 5.74 | 126.81 | 122.80 |
| 1 | YA | 1030 | G | N9-C4-C5 | -5.72 | 103.11 | 105.40 |
| 32 | XA | 88 | A | N9-C4-C5 | -5.72 | 103.51 | 105.80 |
| 4 | YE | 52 | LEU | CA-CB-CG | 5.71 | 128.44 | 115.30 |
| 32 | QA | 1137 | C | C6-N1-C2 | -5.69 | 118.03 | 120.30 |
| 1 | RA | 847 | U | C2-N1-C1' | 5.67 | 124.50 | 117.70 |
| 1 | YA | 887 | A | O4'-C1'-N9 | 5.67 | 112.73 | 108.20 |
| 32 | XA | 1158 | C | C5-C6-N1 | 5.67 | 123.83 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | YA | 1530 | C | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 1 | YA | 847 | U | C2-N1-C1' | 5.64 | 124.47 | 117.70 |
| 1 | RA | 1530 | C | P-O3'-C3' | 5.61 | 126.43 | 119.70 |
| 32 | QA | 1036 | G | C6-C5-N7 | -5.61 | 127.03 | 130.40 |
| 1 | RA | 1050 | A | C5-C6-N6 | 5.58 | 128.16 | 123.70 |
| 7 | YH | 69 | ARG | NE-CZ-NH1 | -5.58 | 117.51 | 120.30 |
| 1 | YA | 1091 | G | N3-C4-C5 | -5.55 | 125.83 | 128.60 |
| 32 | XA | 1054 | C | N3-C2-O2 | -5.55 | 118.02 | 121.90 |
| 1 | RA | 1091 | G | N3-C4-C5 | -5.54 | 125.83 | 128.60 |
| 32 | XA | 1256 | A | O4'-C1'-N9 | -5.54 | 103.77 | 108.20 |
| 1 | YA | 1052 | C | C2-N1-C1' | 5.53 | 124.89 | 118.80 |
| 1 | RA | 1992 | G | P-O3'-C3' | 5.53 | 126.34 | 119.70 |
| 32 | QA | 1205 | U | N3-C4-O4 | -5.52 | 115.54 | 119.40 |
| 1 | RA | 2187 | G | N3-C4-N9 | 5.52 | 129.31 | 126.00 |
| 1 | RA | 1313 | U | C2-N1-C1' | 5.51 | 124.31 | 117.70 |
| 1 | RA | 1076 | C | OP1-P-O3' | 5.50 | 117.29 | 105.20 |
| 1 | RA | 1210 | A | P-O3'-C3' | 5.49 | 126.29 | 119.70 |
| 32 | QA | 993 | G | C4-N9-C1' | 5.49 | 133.64 | 126.50 |
| 1 | YA | 277 | C | N3-C4-C5 | 5.47 | 124.09 | 121.90 |
| 32 | QA | 1330 | U | O5'-P-OP1 | 5.46 | 117.25 | 110.70 |
| 1 | RA | 2573 | C | C5-C4-N4 | -5.45 | 116.38 | 120.20 |
| 1 | YA | 2573 | C | C4-C5-C6 | -5.43 | 114.69 | 117.40 |
| 1 | YA | 1028 | A | C5-C6-N6 | -5.42 | 119.36 | 123.70 |
| 32 | QA | 993 | G | N3-C4-C5 | -5.41 | 125.90 | 128.60 |
| 32 | QA | 1201 | A | P-O3'-C3' | 5.41 | 126.19 | 119.70 |
| 32 | QA | 839 | U | P-O3'-C3' | 5.40 | 126.18 | 119.70 |
| 1 | YA | 1050 | A | C4-C5-N7 | 5.40 | 113.40 | 110.70 |
| 32 | QA | 266 | G | P-O3'-C3' | 5.39 | 126.17 | 119.70 |
| 32 | XA | 60 | A | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 1 | RA | 847 | U | N1-C2-O2 | 5.37 | 126.56 | 122.80 |
| 1 | RA | 2187 | G | N9-C4-C5 | -5.37 | 103.25 | 105.40 |
| 1 | RA | 2218 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 1 | YA | 277 | C | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 7 | YH | 88 | LEU | CA-CB-CG | 5.34 | 127.59 | 115.30 |
| 1 | YA | 1992 | G | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 1 | YA | 1052 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 1 | RA | 2573 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | YA | 614(A) | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 32 | QA | 991 | U | P-O3'-C3' | 5.33 | 126.10 | 119.70 |
| 32 | XA | 88 | A | C4-C5-N7 | 5.32 | 113.36 | 110.70 |
| 1 | RA | 748 | G | C8-N9-C1' | 5.31 | 133.90 | 127.00 |
| 32 | QA | 1022 | G | N3-C4-N9 | 5.31 | 129.19 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 32 | XA | 748 | C | P-O3'-C3' | 5.30 | 126.06 | 119.70 |
| 1 | RA | 2465 | C | C2-N1-C1' | 5.30 | 124.63 | 118.80 |
| 32 | XA | 1025 | U | C5-C6-N1 | -5.29 | 120.06 | 122.70 |
| 32 | QA | 975 | A | O4'-C1'-N9 | -5.25 | 104.00 | 108.20 |
| 32 | QA | 1022 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | RA | 2603 | G | C4-N9-C1' | -5.22 | 119.71 | 126.50 |
| 32 | QA | 754 | C | C2-N1-C1' | 5.22 | 124.54 | 118.80 |
| 32 | QA | 1442(A) | G | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 1 | YA | 2603 | G | N3-C4-C5 | 5.22 | 131.21 | 128.60 |
| 1 | RA | 1914 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 1 | RA | 1053 | C | P-O3'-C3' | 5.21 | 125.95 | 119.70 |
| 32 | QA | 365 | U | C2-N1-C1' | 5.21 | 123.95 | 117.70 |
| 1 | YA | 847 | U | N3-C2-O2 | -5.19 | 118.56 | 122.20 |
| 1 | RA | 1052 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 1 | YA | 614(A) | U | N1-C2-O2 | 5.18 | 126.43 | 122.80 |
| 1 | YA | 2318 | G | C4-N9-C1' | 5.18 | 133.24 | 126.50 |
| 32 | QA | 442 | C | C2-N1-C1' | 5.18 | 124.50 | 118.80 |
| 32 | QA | 254 | G | O5'-P-OP1 | -5.18 | 101.04 | 105.70 |
| 1 | RA | 2603 | G | C8-N9-C1' | 5.17 | 133.72 | 127.00 |
| 1 | RA | 887 | A | O4'-C1'-N9 | 5.17 | 112.33 | 108.20 |
| 1 | YA | 1126 | A | C5-N7-C8 | 5.16 | 106.48 | 103.90 |
| 1 | YA | 2318 | G | N3-C4-C5 | -5.15 | 126.02 | 128.60 |
| 32 | QA | 266 | G | O4'-C1'-N9 | -5.15 | 104.08 | 108.20 |
| 1 | YA | 859 | G | N3-C4-C5 | 5.15 | 131.17 | 128.60 |
| 32 | QA | 365 | U | O4'-C1'-N1 | 5.14 | 112.31 | 108.20 |
| 1 | YA | 1028 | A | C6-N1-C2 | -5.14 | 115.52 | 118.60 |
| 1 | YA | 1053 | C | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 32 | QA | 1137 | C | C5-C6-N1 | 5.11 | 123.55 | 121.00 |
| 1 | RA | 748 | G | C4-N9-C1' | -5.10 | 119.87 | 126.50 |
| 1 | YA | 2318 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 1 | RA | 1313 | U | N1-C2-O2 | 5.10 | 126.37 | 122.80 |
| 1 | RA | 1372 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 32 | XA | 1067 | A | P-O3'-C3' | 5.08 | 125.80 | 119.70 |
| 1 | RA | 1076 | C | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 32 | XA | 1442(A) | G | P-O3'-C3' | 5.06 | 125.78 | 119.70 |
| 1 | YA | 1029 | A | N9-C4-C5 | 5.06 | 107.82 | 105.80 |
| 1 | YA | 2751 | G | C5-N7-C8 | -5.06 | 101.77 | 104.30 |
| 1 | YA | 301 | G | N3-C4-C5 | 5.05 | 131.13 | 128.60 |
| 32 | XA | 1442(A) | G | C4-N9-C1' | 5.05 | 133.06 | 126.50 |
| 1 | YA | 1125 | G | C4-N9-C1' | 5.04 | 133.05 | 126.50 |
| 32 | QA | 1065 | U | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | YA | 2465 | C | N3-C2-O2 | -5.04 | 118.37 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | RA | 2104 | G | N3-C4-C5 | -5.03 | 126.08 | 128.60 |
| 32 | QA | 1030(A) | C | C5-C4-N4 | -5.03 | 116.68 | 120.20 |
| 32 | XA | 1003 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 1 | RA | 2186 | G | C8-N9-C1' | 5.00 | 133.50 | 127.00 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 33 | QB | 231 | GLU | Peptide |
| 26 | R4 | 67 | TYR | Peptide |
| 14 | RS | 58 | LEU | Peptide |
| 43 | XL | 86 | ARG | 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 | RA | 61758 | 0 | 31145 | 564 | 0 |
| 1 | YA | 61758 | 0 | 31148 | 595 | 1 |
| 2 | RB | 2572 | 0 | 1305 | 8 | 0 |
| 2 | YB | 2573 | 0 | 1306 | 23 | 0 |
| 3 | RD | 2131 | 0 | 2207 | 42 | 0 |
| 3 | YD | 2136 | 0 | 2218 | 37 | 0 |
| 4 | RE | 1559 | 0 | 1618 | 27 | 0 |
| 4 | YE | 1559 | 0 | 1618 | 30 | 0 |
| 5 | RF | 1584 | 0 | 1625 | 31 | 0 |
| 5 | YF | 1580 | 0 | 1619 | 42 | 0 |
| 6 | RG | 1426 | 0 | 1445 | 34 | 0 |
| 6 | YG | 1424 | 0 | 1441 | 45 | 0 |
| 7 | RH | 1330 | 0 | 1407 | 24 | 0 |
| 7 | YH | 1324 | 0 | 1402 | 36 | 0 |
| 8 | RI | 1094 | 0 | 1127 | 23 | 0 |
| 8 | YI | 1076 | 0 | 1094 | 21 | 0 |
| 9 | RN | 1121 | 0 | 1195 | 14 | 0 |
| 9 | YN | 1117 | 0 | 1184 | 21 | 0 |
| 10 | RO | 933 | 0 | 996 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | YO | 933 | 0 | 996 | 10 | 0 |
| 11 | RP | 1135 | 0 | 1212 | 25 | 0 |
| 11 | YP | 1135 | 0 | 1212 | 32 | 0 |
| 12 | RQ | 1122 | 0 | 1179 | 22 | 0 |
| 12 | YQ | 1122 | 0 | 1179 | 20 | 0 |
| 13 | RR | 968 | 0 | 1033 | 15 | 0 |
| 13 | YR | 968 | 0 | 1033 | 11 | 0 |
| 14 | RS | 877 | 0 | 938 | 9 | 0 |
| 14 | YS | 870 | 0 | 923 | 14 | 0 |
| 15 | RT | 1091 | 0 | 1151 | 21 | 0 |
| 15 | YT | 1083 | 0 | 1136 | 19 | 0 |
| 16 | RU | 959 | 0 | 1019 | 12 | 0 |
| 16 | YU | 959 | 0 | 1019 | 13 | 0 |
| 17 | RV | 775 | 0 | 841 | 7 | 0 |
| 17 | YV | 771 | 0 | 830 | 15 | 0 |
| 18 | RW | 886 | 0 | 940 | 13 | 0 |
| 18 | YW | 886 | 0 | 940 | 8 | 0 |
| 19 | RX | 750 | 0 | 814 | 17 | 0 |
| 19 | YX | 750 | 0 | 814 | 12 | 0 |
| 20 | RY | 810 | 0 | 892 | 14 | 0 |
| 20 | YY | 810 | 0 | 888 | 18 | 0 |
| 21 | RZ | 1485 | 0 | 1493 | 19 | 0 |
| 21 | YZ | 1469 | 0 | 1467 | 26 | 0 |
| 22 | R0 | 608 | 0 | 622 | 10 | 0 |
| 22 | Y0 | 608 | 0 | 622 | 14 | 0 |
| 23 | R1 | 754 | 0 | 823 | 10 | 0 |
| 23 | Y1 | 759 | 0 | 837 | 20 | 0 |
| 24 | R2 | 588 | 0 | 643 | 5 | 1 |
| 24 | Y2 | 592 | 0 | 654 | 7 | 0 |
| 25 | R3 | 469 | 0 | 518 | 4 | 0 |
| 25 | Y3 | 464 | 0 | 514 | 7 | 0 |
| 26 | R4 | 546 | 0 | 522 | 26 | 0 |
| 26 | Y4 | 536 | 0 | 514 | 28 | 0 |
| 27 | R5 | 459 | 0 | 476 | 11 | 0 |
| 27 | Y5 | 455 | 0 | 465 | 7 | 0 |
| 28 | R6 | 453 | 0 | 473 | 14 | 0 |
| 28 | Y6 | 449 | 0 | 469 | 4 | 0 |
| 29 | R7 | 418 | 0 | 467 | 13 | 0 |
| 29 | Y7 | 418 | 0 | 467 | 8 | 0 |
| 30 | R8 | 517 | 0 | 582 | 21 | 0 |
| 30 | Y8 | 517 | 0 | 582 | 17 | 0 |
| 31 | R9 | 307 | 0 | 335 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31 | Y9 | 307 | 0 | 335 | 15 | 0 |
| 32 | QA | 32246 | 0 | 16294 | 310 | 0 |
| 32 | XA | 32331 | 0 | 16338 | 344 | 0 |
| 33 | QB | 1842 | 0 | 1862 | 55 | 0 |
| 33 | XB | 1825 | 0 | 1828 | 57 | 0 |
| 34 | QC | 1558 | 0 | 1557 | 30 | 0 |
| 34 | XC | 1542 | 0 | 1517 | 38 | 0 |
| 35 | QD | 1665 | 0 | 1688 | 42 | 0 |
| 35 | XD | 1668 | 0 | 1704 | 39 | 0 |
| 36 | QE | 1133 | 0 | 1191 | 31 | 0 |
| 36 | XE | 1133 | 0 | 1191 | 24 | 0 |
| 37 | QF | 814 | 0 | 808 | 14 | 0 |
| 37 | XF | 816 | 0 | 808 | 11 | 0 |
| 38 | QG | 1235 | 0 | 1249 | 20 | 0 |
| 38 | XG | 1229 | 0 | 1238 | 16 | 0 |
| 39 | QH | 1098 | 0 | 1143 | 26 | 0 |
| 39 | XH | 1088 | 0 | 1126 | 14 | 0 |
| 40 | QI | 986 | 0 | 990 | 28 | 0 |
| 40 | XI | 966 | 0 | 953 | 37 | 0 |
| 41 | QJ | 719 | 0 | 672 | 22 | 0 |
| 41 | XJ | 710 | 0 | 661 | 30 | 0 |
| 42 | QK | 834 | 0 | 838 | 15 | 0 |
| 42 | XK | 833 | 0 | 836 | 12 | 0 |
| 43 | QL | 932 | 0 | 980 | 14 | 0 |
| 43 | XL | 932 | 0 | 981 | 20 | 0 |
| 44 | QM | 914 | 0 | 954 | 30 | 0 |
| 44 | XM | 895 | 0 | 920 | 24 | 0 |
| 45 | QN | 492 | 0 | 529 | 19 | 0 |
| 45 | XN | 492 | 0 | 529 | 19 | 0 |
| 46 | QO | 728 | 0 | 760 | 17 | 0 |
| 46 | XO | 728 | 0 | 760 | 9 | 0 |
| 47 | QP | 681 | 0 | 697 | 11 | 0 |
| 47 | XP | 677 | 0 | 686 | 19 | 0 |
| 48 | QQ | 823 | 0 | 891 | 12 | 0 |
| 48 | XQ | 823 | 0 | 891 | 7 | 0 |
| 49 | QR | 555 | 0 | 618 | 11 | 0 |
| 49 | XR | 555 | 0 | 618 | 14 | 0 |
| 50 | QS | 648 | 0 | 658 | 16 | 0 |
| 50 | XS | 645 | 0 | 635 | 27 | 0 |
| 51 | QT | 732 | 0 | 809 | 16 | 0 |
| 51 | XT | 733 | 0 | 795 | 15 | 0 |
| 52 | QU | 199 | 0 | 208 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 52 | XU | 199 | 0 | 208 | 7 | 0 |
| 53 | QV | 1644 | 0 | 835 | 23 | 0 |
| 53 | XV | 1644 | 0 | 836 | 15 | 0 |
| 54 | QX | 215 | 0 | 109 | 1 | 0 |
| 54 | XX | 193 | 0 | 97 | 5 | 0 |
| 55 | QY | 2014 | 0 | 1981 | 60 | 0 |
| 55 | XY | 2023 | 0 | 1988 | 78 | 0 |
| 56 | QA | 256 | 0 | 0 | 0 | 0 |
| 56 | QB | 1 | 0 | 0 | 0 | 0 |
| 56 | QD | 3 | 0 | 0 | 0 | 0 |
| 56 | QE | 2 | 0 | 0 | 0 | 0 |
| 56 | QF | 1 | 0 | 0 | 0 | 0 |
| 56 | QG | 2 | 0 | 0 | 0 | 0 |
| 56 | QH | 1 | 0 | 0 | 0 | 0 |
| 56 | QI | 1 | 0 | 0 | 0 | 0 |
| 56 | QL | 2 | 0 | 0 | 0 | 0 |
| 56 | QM | 1 | 0 | 0 | 0 | 0 |
| 56 | QN | 2 | 0 | 0 | 0 | 0 |
| 56 | QO | 1 | 0 | 0 | 0 | 0 |
| 56 | QQ | 1 | 0 | 0 | 0 | 0 |
| 56 | QR | 1 | 0 | 0 | 0 | 0 |
| 56 | QT | 2 | 0 | 0 | 0 | 0 |
| 56 | QV | 6 | 0 | 0 | 0 | 0 |
| 56 | R0 | 4 | 0 | 0 | 0 | 0 |
| 56 | R1 | 4 | 0 | 0 | 0 | 0 |
| 56 | R3 | 2 | 0 | 0 | 0 | 0 |
| 56 | R5 | 3 | 0 | 0 | 0 | 0 |
| 56 | R7 | 2 | 0 | 0 | 0 | 0 |
| 56 | R8 | 1 | 0 | 0 | 0 | 0 |
| 56 | RA | 1039 | 0 | 0 | 0 | 0 |
| 56 | RB | 27 | 0 | 0 | 0 | 0 |
| 56 | RD | 15 | 0 | 0 | 0 | 0 |
| 56 | RE | 8 | 0 | 0 | 0 | 0 |
| 56 | RF | 12 | 0 | 0 | 0 | 0 |
| 56 | RG | 4 | 0 | 0 | 0 | 0 |
| 56 | RH | 1 | 0 | 0 | 0 | 0 |
| 56 | RN | 2 | 0 | 0 | 0 | 0 |
| 56 | RO | 1 | 0 | 0 | 0 | 0 |
| 56 | RP | 1 | 0 | 0 | 0 | 0 |
| 56 | RQ | 6 | 0 | 0 | 0 | 0 |
| 56 | RR | 3 | 0 | 0 | 0 | 0 |
| 56 | RT | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | RU | 2 | 0 | 0 | 0 | 0 |
| 56 | RV | 4 | 0 | 0 | 0 | 0 |
| 56 | RW | 2 | 0 | 0 | 0 | 0 |
| 56 | RX | 1 | 0 | 0 | 0 | 0 |
| 56 | RY | 1 | 0 | 0 | 0 | 0 |
| 56 | RZ | 1 | 0 | 0 | 0 | 0 |
| 56 | XA | 183 | 0 | 0 | 0 | 0 |
| 56 | XE | 1 | 0 | 0 | 0 | 0 |
| 56 | XF | 2 | 0 | 0 | 0 | 0 |
| 56 | XJ | 1 | 0 | 0 | 0 | 0 |
| 56 | XK | 1 | 0 | 0 | 0 | 0 |
| 56 | XL | 1 | 0 | 0 | 0 | 0 |
| 56 | XR | 1 | 0 | 0 | 0 | 0 |
| 56 | XT | 1 | 0 | 0 | 0 | 0 |
| 56 | XV | 4 | 0 | 0 | 0 | 0 |
| 56 | XX | 1 | 0 | 0 | 0 | 0 |
| 56 | Y0 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y1 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y7 | 2 | 0 | 0 | 0 | 0 |
| 56 | Y8 | 2 | 0 | 0 | 0 | 0 |
| 56 | YA | 744 | 0 | 0 | 0 | 0 |
| 56 | YB | 18 | 0 | 0 | 0 | 0 |
| 56 | YD | 9 | 0 | 0 | 0 | 0 |
| 56 | YE | 5 | 0 | 0 | 0 | 0 |
| 56 | YF | 3 | 0 | 0 | 0 | 0 |
| 56 | YG | 2 | 0 | 0 | 0 | 0 |
| 56 | YI | 1 | 0 | 0 | 0 | 0 |
| 56 | YN | 1 | 0 | 0 | 0 | 0 |
| 56 | YO | 2 | 0 | 0 | 0 | 0 |
| 56 | YP | 1 | 0 | 0 | 0 | 0 |
| 56 | YQ | 2 | 0 | 0 | 0 | 0 |
| 56 | YR | 1 | 0 | 0 | 0 | 0 |
| 56 | YT | 4 | 0 | 0 | 0 | 0 |
| 56 | YV | 1 | 0 | 0 | 0 | 0 |
| 56 | YW | 2 | 0 | 0 | 0 | 0 |
| 56 | YX | 1 | 0 | 0 | 0 | 0 |
| 57 | QN | 1 | 0 | 0 | 0 | 0 |
| 57 | R4 | 1 | 0 | 0 | 0 | 0 |
| 57 | R5 | 1 | 0 | 0 | 0 | 0 |
| 57 | R6 | 1 | 0 | 0 | 0 | 0 |
| 57 | R9 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57 | RY | 1 | 0 | 0 | 0 | 0 |
| 57 | XN | 1 | 0 | 0 | 0 | 0 |
| 57 | Y4 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y6 | 1 | 0 | 0 | 0 | 0 |
| 57 | Y9 | 1 | 0 | 0 | 0 | 0 |
| 57 | YY | 1 | 0 | 0 | 0 | 0 |
| 58 | QD | 8 | 0 | 0 | 0 | 0 |
| 58 | XD | 8 | 0 | 0 | 0 | 0 |
| All | All | 294739 | 0 | 198434 | 3343 | 1 |

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 7.

All (3343) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:YA:2552:2MU:C5 | 1:YA:2552:2MU:C4 | 1.80 | 1.59 |
| 1:RA:2552:2MU:C4 | 1:RA:2552:2MU:C5 | 1.80 | 1.58 |
| 32:XA:1003:G:H2' | 32:XA:1004:A:H4' | 1.32 | 1.08 |
| 1:YA:1029:A:N6 | 1:YA:1125:G:O2' | 1.87 | 1.06 |
| 26:Y4:59:PHE:HA | 26:Y4:61:ARG:N | 1.76 | 1.00 |
| 26:Y4:59:PHE:HA | 26:Y4:61:ARG:H | 1.28 | 0.99 |
| 1:YA:2131:G:H5'' | 1:YA:2132:U:H5' | 1.45 | 0.98 |
| 10:RO:48:PRO:HB3 | 32:QA:1422:G:H5'' | 1.46 | 0.97 |
| 1:RA:2131:G:H5'' | 1:RA:2132:U:H5' | 1.45 | 0.97 |
| 1:RA:2285:C:OP2 | 28:R6:29:ASN:ND2 | 1.99 | 0.94 |
| 15:RT:55:ASN:H | 15:RT:59:THR:HG22 | 1.31 | 0.92 |
| 14:RS:59:LYS:HD2 | 14:RS:60:GLY:H | 1.30 | 0.92 |
| 1:YA:2128:C:H42 | 1:YA:2160:G:H1 | 1.17 | 0.91 |
| 40:QI:17:VAL:HG21 | 40:QI:81:ILE:HG22 | 1.53 | 0.90 |
| 1:RA:2128:C:H42 | 1:RA:2160:G:H1 | 1.15 | 0.90 |
| 10:YO:48:PRO:HB3 | 32:XA:1422:G:H5'' | 1.52 | 0.90 |
| 1:RA:2573:C:N4 | 55:QY:241:ASP:OD1 | 2.05 | 0.89 |
| 1:YA:1041:C:H42 | 1:YA:1114:G:H1 | 1.19 | 0.89 |
| 6:RG:179:PRO:HB2 | 26:R4:42:PHE:HE2 | 1.37 | 0.89 |
| 1:RA:250:G:OP2 | 30:R8:13:ARG:NH2 | 2.06 | 0.89 |
| 33:XB:15:VAL:HB | 33:XB:209:ARG:HB3 | 1.53 | 0.88 |
| 32:QA:78:G:H1 | 32:QA:91:C:H42 | 1.22 | 0.87 |
| 32:XA:1493:A:H4' | 55:XY:121:GLY:H | 1.39 | 0.87 |
| 32:QA:975:A:H4' | 32:QA:976:G:H5'' | 1.58 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:RA:1041:C:H42 | 1:RA:1114:G:H1 | 1.24 | 0.85 |
| 50:XS:50:ALA:HB1 | 50:XS:57:HIS:HB3 | 1.57 | 0.85 |
| 8:YI:92:VAL:HG23 | 8:YI:120:ILE:HB | 1.58 | 0.85 |
| 32:XA:390:C:O3' | 47:XP:28:ARG:NH2 | 2.11 | 0.83 |
| 1:YA:1028:A:HO2' | 1:YA:2486:G:HO2' | 1.18 | 0.83 |
| 35:XD:18:LYS:NZ | 35:XD:31:CYS:SG | 2.51 | 0.83 |
| 5:YF:178:PRO:HB2 | 5:YF:201:VAL:HG21 | 1.60 | 0.83 |
| 55:XY:200:ALA:HB3 | 55:XY:302:ASP:HB3 | 1.60 | 0.83 |
| 1:YA:250:G:OP2 | 30:Y8:13:ARG:NH2 | 2.11 | 0.83 |
| 4:RE:47:VAL:HG21 | 4:RE:86:PRO:HD2 | 1.60 | 0.82 |
| 44:XM:107:ALA:HB3 | 44:XM:111:LYS:HD2 | 1.61 | 0.82 |
| 6:YG:136:ARG:HG2 | 6:YG:137:GLU:HG3 | 1.60 | 0.82 |
| 1:YA:2452:C:H4' | 55:XY:239:THR:HG21 | 1.61 | 0.82 |
| 4:YE:47:VAL:HG11 | 4:YE:86:PRO:HD2 | 1.60 | 0.82 |
| 29:R7:34:ARG:NH1 | 29:R7:41:ARG:O | 2.13 | 0.81 |
| 1:RA:2552:2MU:C4 | 1:RA:2552:2MU:C6 | 2.54 | 0.81 |
| 1:YA:2753:A:N3 | 31:Y9:15:LYS:NZ | 2.28 | 0.81 |
| 10:RO:35:VAL:HG11 | 10:RO:103:ALA:HB3 | 1.62 | 0.81 |
| 32:XA:975:A:H4' | 32:XA:976:G:H5'' | 1.60 | 0.81 |
| 41:XJ:49:VAL:HG23 | 45:YN:41:ARG:HB2 | 1.62 | 0.81 |
| 40:XI:53:VAL:O | 40:XI:55:ALA:N | 2.13 | 0.81 |
| 1:YA:1038:C:H42 | 1:YA:1117:G:H1 | 1.28 | 0.81 |
| 1:YA:833:U:O2 | 11:YP:55:ARG:NH2 | 2.14 | 0.81 |
| 1:YA:1028:A:O2' | 1:YA:2486:G:O2' | 1.98 | 0.80 |
| 1:RA:1798:U:H5' | 3:RD:259:THR:HG22 | 1.63 | 0.80 |
| 15:YT:16:ARG:NH2 | 15:YT:83:ILE:O | 2.14 | 0.80 |
| 32:QA:664:G:H22 | 32:QA:741:G:H1 | 1.30 | 0.80 |
| 32:QA:538:G:H5'' | 43:QL:114:LYS:HB2 | 1.64 | 0.79 |
| 1:RA:83:G:OP1 | 20:RY:95:LYS:NZ | 2.15 | 0.79 |
| 27:Y5:16:ARG:NH1 | 27:Y5:17:ASP:OD1 | 2.16 | 0.79 |
| 1:YA:2748:A:H5' | 7:YH:4:ILE:HD12 | 1.63 | 0.79 |
| 4:YE:12:THR:HG23 | 15:YT:58:ASN:HD21 | 1.48 | 0.79 |
| 1:RA:956:G:OP2 | 12:RQ:14:ARG:NH2 | 2.16 | 0.79 |
| 32:QA:1189:C:OP1 | 41:QJ:51:ARG:NH2 | 2.15 | 0.78 |
| 32:QA:532:A:H61 | 34:QC:193:TYR:HA | 1.49 | 0.78 |
| 42:QK:48:ILE:HD12 | 42:QK:63:LEU:HB2 | 1.65 | 0.78 |
| 1:YA:2756:U:H5'' | 31:Y9:19:ARG:HA | 1.65 | 0.78 |
| 1:YA:1798:U:OP2 | 3:YD:274:ARG:NH2 | 2.16 | 0.78 |
| 10:YO:35:VAL:HG11 | 10:YO:103:ALA:HB3 | 1.66 | 0.78 |
| 50:XS:20:LEU:HD23 | 50:XS:23:ASN:HD22 | 1.47 | 0.78 |
| 1:RA:272(K):U:H1' | 8:RI:50:ARG:HH21 | 1.46 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:QB:21:ARG:HH22 | 33:QB:23:ARG:HH21 | 1.32 | 0.78 |
| 1:RA:2343:C:HO2' | 1:RA:2373:G:HO2' | 1.32 | 0.78 |
| 33:XB:88:ALA:HB1 | 33:XB:222:ILE:HD11 | 1.65 | 0.77 |
| 1:YA:530:G:N1 | 1:YA:2023:G:OP1 | 2.16 | 0.77 |
| 48:XQ:66:SER:O | 48:XQ:70:ARG:NH1 | 2.18 | 0.77 |
| 1:RA:1250:G:N7 | 11:RP:18:ARG:NH2 | 2.32 | 0.77 |
| 14:YS:50:SER:O | 14:YS:76:LYS:NZ | 2.14 | 0.77 |
| 32:XA:1314:C:OP2 | 50:XS:4:SER:OG | 2.03 | 0.76 |
| 32:QA:1183:A:O2' | 32:QA:1184:G:OP1 | 2.03 | 0.76 |
| 18:RW:14:PRO:HG2 | 18:RW:78:GLU:HG2 | 1.67 | 0.76 |
| 21:YZ:45:ASP:OD1 | 21:YZ:49:ARG:NH1 | 2.18 | 0.76 |
| 1:RA:1036:G:OP2 | 7:RH:59:ARG:NH1 | 2.19 | 0.76 |
| 1:RA:2140:C:H2' | 1:RA:2141:G:H8 | 1.51 | 0.76 |
| 40:QI:50:LEU:HD13 | 40:QI:56:LEU:HA | 1.66 | 0.75 |
| 32:QA:189(B):C:H42 | 32:QA:189(K):G:H1 | 1.33 | 0.75 |
| 6:RG:161:THR:HG22 | 6:RG:163:ALA:H | 1.51 | 0.75 |
| 41:QJ:49:VAL:HG23 | 45:QN:41:ARG:HB2 | 1.67 | 0.75 |
| 55:QY:242:SER:HA | 55:QY:263:GLN:HB3 | 1.68 | 0.75 |
| 32:QA:38:G:H22 | 32:QA:397:A:H5' | 1.52 | 0.75 |
| 41:XJ:17:ASP:OD1 | 41:XJ:70:ARG:NH1 | 2.19 | 0.75 |
| 1:YA:1051:G:H4' | 1:YA:2752:C:H4' | 1.68 | 0.75 |
| 27:R5:40:LYS:NZ | 27:R5:44:THR:O | 2.18 | 0.75 |
| 51:QT:86:ARG:O | 51:QT:90:GLN:NE2 | 2.20 | 0.74 |
| 53:XV:75:C:OP2 | 55:XY:261:ARG:NH2 | 2.18 | 0.74 |
| 1:YA:958:U:OP2 | 12:YQ:14:ARG:NH1 | 2.19 | 0.74 |
| 26:R4:59:PHE:HZ | 50:QS:45:VAL:HG21 | 1.50 | 0.74 |
| 1:YA:1815:A:OP2 | 3:YD:54:ARG:NH2 | 2.20 | 0.74 |
| 19:YX:88:LYS:HE2 | 19:YX:93:GLU:HG3 | 1.69 | 0.74 |
| 55:QY:217:ILE:HD11 | 55:QY:222:LEU:HD21 | 1.69 | 0.74 |
| 32:QA:159:G:N2 | 32:QA:162:A:OP2 | 2.15 | 0.74 |
| 1:RA:631:A:OP1 | 11:RP:65:ARG:NH1 | 2.19 | 0.74 |
| 1:YA:1062:G:H5' | 1:YA:1070:A:H5'' | 1.67 | 0.74 |
| 28:R6:24:GLU:OE2 | 30:R8:34:TRP:NE1 | 2.19 | 0.74 |
| 1:RA:1049:C:N4 | 1:RA:2751:G:O6 | 2.19 | 0.74 |
| 55:QY:315:GLY:HA2 | 55:QY:329:LEU:HD12 | 1.70 | 0.74 |
| 32:XA:642:A:N3 | 39:XH:113:SER:OG | 2.20 | 0.73 |
| 35:QD:18:LYS:NZ | 35:QD:31:CYS:SG | 2.61 | 0.73 |
| 44:XM:58:GLU:O | 44:XM:62:ASN:ND2 | 2.21 | 0.73 |
| 55:XY:183:ARG:HB3 | 55:XY:309:THR:HG22 | 1.68 | 0.73 |
| 20:RY:92:ASN:HB2 | 20:RY:94:LYS:H | 1.51 | 0.73 |
| 1:RA:1038:C:H42 | 1:RA:1117:G:H1 | 1.35 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:XA:1047:G:H5'' | 45:XN:4:LYS:HD3 | 1.68 | 0.73 |
| 6:YG:161:THR:HG22 | 6:YG:163:ALA:H | 1.53 | 0.73 |
| 32:QA:201:C:H42 | 32:QA:216:G:H1 | 1.35 | 0.73 |
| 22:R0:10:THR:HG22 | 22:R0:12:ASN:H | 1.53 | 0.73 |
| 32:QA:1279:A:O2' | 32:QA:1281:U:OP2 | 2.07 | 0.73 |
| 3:RD:69:ARG:NH2 | 3:RD:128:GLY:O | 2.22 | 0.73 |
| 15:RT:35:LYS:HG2 | 15:RT:40:THR:HG22 | 1.71 | 0.73 |
| 34:XC:109:PRO:HB3 | 34:XC:115:LEU:HD23 | 1.71 | 0.73 |
| 1:YA:2140:C:H2' | 1:YA:2141:G:H8 | 1.52 | 0.72 |
| 1:RA:1062:G:H5' | 1:RA:1070:A:H5'' | 1.70 | 0.72 |
| 1:YA:1071:G:N2 | 1:YA:1089:G:O6 | 2.15 | 0.72 |
| 1:RA:2384:G:OP2 | 22:R0:55:ARG:NH1 | 2.22 | 0.72 |
| 44:XM:98:VAL:HG23 | 44:XM:110:ARG:HH12 | 1.55 | 0.72 |
| 55:QY:177:PHE:O | 55:QY:321:ARG:NH1 | 2.20 | 0.72 |
| 1:RA:1971:A:OP2 | 3:RD:242:ARG:NH2 | 2.20 | 0.72 |
| 1:RA:994:C:OP1 | 16:RU:53:ARG:NH2 | 2.23 | 0.72 |
| 32:XA:1189:C:OP1 | 41:XJ:51:ARG:NH2 | 2.22 | 0.72 |
| 22:Y0:11:ARG:O | 22:Y0:14:ARG:NH2 | 2.22 | 0.72 |
| 32:XA:955:U:OP1 | 55:XY:137:ARG:NH1 | 2.22 | 0.72 |
| 2:YB:105:A:OP1 | 21:YZ:72:ARG:NH1 | 2.21 | 0.72 |
| 35:QD:148:VAL:HG11 | 35:QD:158:ILE:HD12 | 1.70 | 0.71 |
| 41:QJ:35:SER:HB3 | 41:QJ:73:ASP:HB2 | 1.70 | 0.71 |
| 47:QP:53:VAL:HG13 | 47:QP:79:VAL:HG12 | 1.72 | 0.71 |
| 55:QY:248:HIS:HB2 | 55:QY:274:LEU:HD11 | 1.70 | 0.71 |
| 22:R0:11:ARG:O | 22:R0:14:ARG:NH2 | 2.19 | 0.71 |
| 21:RZ:72:ARG:HG2 | 21:RZ:89:PHE:HB2 | 1.72 | 0.71 |
| 3:RD:71:ASP:HB3 | 3:RD:103:ARG:HH22 | 1.55 | 0.71 |
| 15:RT:16:ARG:NH2 | 15:RT:83:ILE:O | 2.23 | 0.71 |
| 55:XY:208:GLU:HG2 | 55:XY:210:PRO:HD3 | 1.72 | 0.71 |
| 1:YA:2134:A:N6 | 1:YA:2156:G:O2' | 2.23 | 0.71 |
| 11:YP:59:LEU:HD11 | 30:Y8:10:ALA:HB2 | 1.69 | 0.71 |
| 7:YH:7:LEU:O | 7:YH:69:ARG:NH1 | 2.23 | 0.71 |
| 17:YV:6:LYS:HB2 | 17:YV:38:LEU:HD21 | 1.69 | 0.71 |
| 32:QA:316:G:OP2 | 32:QA:351:G:O2' | 2.09 | 0.71 |
| 10:RO:97:ARG:NH1 | 32:QA:339:C:OP2 | 2.23 | 0.71 |
| 50:QS:41:VAL:HG12 | 50:QS:44:MET:HG3 | 1.72 | 0.71 |
| 6:YG:66:GLN:HG3 | 26:Y4:1:MET:HE3 | 1.72 | 0.71 |
| 6:RG:41:GLN:HB3 | 6:RG:43:LEU:HD13 | 1.72 | 0.71 |
| 34:XC:58:GLU:HB3 | 41:XJ:92:THR:HG21 | 1.72 | 0.71 |
| 1:YA:2573:C:N4 | 55:XY:239:THR:HA | 2.04 | 0.71 |
| 1:YA:1530:C:O2' | 1:YA:1531:C:O5' | 2.07 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:XA:538:G:H5'' | 43:XL:114:LYS:HB2 | 1.73 | 0.71 |
| 1:YA:1028:A:N6 | 1:YA:1126:A:OP1 | 2.19 | 0.71 |
| 1:YA:272(P):C:O2' | 8:YI:42:SER:OG | 2.07 | 0.71 |
| 33:QB:82:ARG:NH1 | 33:QB:86:GLU:OE2 | 2.23 | 0.71 |
| 32:XA:1292:U:OP2 | 38:XG:41:ARG:NH2 | 2.23 | 0.71 |
| 5:YF:24:LEU:HD23 | 5:YF:115:ALA:HA | 1.73 | 0.71 |
| 6:YG:136:ARG:HD3 | 6:YG:136:ARG:H | 1.56 | 0.70 |
| 4:RE:77:ILE:HD13 | 4:RE:195:LEU:HD13 | 1.72 | 0.70 |
| 42:XK:99:GLN:HG2 | 42:XK:105:VAL:HG21 | 1.72 | 0.70 |
| 1:RA:1073:A:H2' | 1:RA:1074:G:H8 | 1.57 | 0.70 |
| 32:XA:992:U:H4' | 32:XA:993:G:O5' | 1.91 | 0.70 |
| 32:XA:1031:G:H2' | 32:XA:1032:G:C8 | 2.26 | 0.70 |
| 26:R4:59:PHE:CZ | 50:QS:45:VAL:HG21 | 2.27 | 0.70 |
| 6:YG:63:ILE:HA | 6:YG:143:GLU:HG3 | 1.74 | 0.70 |
| 1:RA:1141:U:OP1 | 9:RN:25:ARG:NH1 | 2.25 | 0.70 |
| 21:RZ:144:LEU:HD21 | 21:RZ:150:LEU:HD13 | 1.73 | 0.70 |
| 15:RT:56:GLY:O | 15:RT:59:THR:HG23 | 1.92 | 0.70 |
| 11:RP:59:LEU:HD11 | 30:R8:10:ALA:HB2 | 1.72 | 0.69 |
| 55:XY:217:ILE:HD11 | 55:XY:222:LEU:HD21 | 1.73 | 0.69 |
| 1:YA:309:G:N3 | 1:YA:329:G:O2' | 2.24 | 0.69 |
| 32:QA:1003:G:N2 | 32:QA:1004:A:N3 | 2.40 | 0.69 |
| 1:RA:1087:G:H1 | 1:RA:1102:C:H42 | 1.38 | 0.69 |
| 1:YA:1971:A:OP2 | 3:YD:242:ARG:NH2 | 2.24 | 0.69 |
| 1:RA:2128:C:N4 | 1:RA:2160:G:H1 | 1.89 | 0.69 |
| 33:XB:78:GLN:O | 33:XB:94:ASN:ND2 | 2.25 | 0.69 |
| 1:RA:530:G:N1 | 1:RA:2023:G:OP1 | 2.24 | 0.69 |
| 1:RA:20:C:OP1 | 16:RU:22:LYS:NZ | 2.25 | 0.69 |
| 22:Y0:10:THR:HG22 | 22:Y0:12:ASN:H | 1.58 | 0.69 |
| 1:YA:1419:A:N6 | 1:YA:1578:U:O2 | 2.20 | 0.69 |
| 32:QA:1492:A:HO2' | 54:QX:20:A:HO2' | 1.35 | 0.69 |
| 1:RA:1024:G:HO2' | 1:RA:1144:G:HO2' | 1.35 | 0.69 |
| 1:YA:2640:G:O3' | 9:YN:74:ARG:NH2 | 2.16 | 0.69 |
| 1:YA:2304:G:H22 | 1:YA:2312:U:H3 | 1.41 | 0.69 |
| 1:RA:1094:U:OP1 | 1:RA:1096:A:N6 | 2.26 | 0.69 |
| 32:XA:664:G:H22 | 32:XA:741:G:H1 | 1.40 | 0.69 |
| 32:QA:1297:C:O2' | 38:QG:114:ARG:NH2 | 2.26 | 0.69 |
| 1:RA:1073:A:H2' | 1:RA:1074:G:C8 | 2.26 | 0.69 |
| 1:RA:143(A):G:H4' | 19:RX:35:THR:HG21 | 1.74 | 0.69 |
| 32:XA:582:U:OP1 | 46:XO:68:ARG:NH2 | 2.22 | 0.69 |
| 55:QY:255:VAL:HG12 | 55:QY:274:LEU:HD23 | 1.75 | 0.69 |
| 40:XI:16:ARG:HB2 | 40:XI:64:THR:HG22 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:Y4:59:PHE:CZ | 50:XS:64:GLU:HB2 | 2.28 | 0.69 |
| 1:YA:1057:A:N7 | 1:YA:1086:A:H2' | 2.08 | 0.69 |
| 33:XB:47:THR:HA | 33:XB:202:PRO:HG2 | 1.73 | 0.69 |
| 1:RA:1815:A:OP2 | 3:RD:54:ARG:NH2 | 2.27 | 0.68 |
| 32:XA:677:U:H3 | 32:XA:713:G:H22 | 1.38 | 0.68 |
| 5:YF:185:ASP:HA | 5:YF:188:ARG:HD3 | 1.75 | 0.68 |
| 55:QY:328:ARG:HH22 | 55:QY:339:MET:C | 1.96 | 0.68 |
| 6:RG:63:ILE:HA | 6:RG:143:GLU:HG3 | 1.74 | 0.68 |
| 41:XJ:52:GLY:O | 45:XN:41:ARG:NH2 | 2.26 | 0.68 |
| 1:RA:587:C:OP2 | 11:RP:21:ARG:NH2 | 2.25 | 0.68 |
| 1:YA:270:A:OP2 | 1:YA:272(X):G:N1 | 2.18 | 0.68 |
| 1:RA:1024:G:O2' | 1:RA:1144:G:O2' | 2.11 | 0.68 |
| 1:YA:2646:C:OP2 | 1:YA:2732:G:O2' | 2.10 | 0.68 |
| 9:YN:94:HIS:HB3 | 9:YN:97:ARG:HD3 | 1.74 | 0.68 |
| 32:XA:1005:A:OP2 | 32:XA:1024:G:N2 | 2.27 | 0.68 |
| 55:XY:145:ARG:HB3 | 55:XY:167:SER:HB2 | 1.75 | 0.68 |
| 26:R4:50:VAL:HG11 | 44:QM:65:LYS:HA | 1.75 | 0.68 |
| 1:YA:855:G:O2' | 22:Y0:27:GLU:OE2 | 2.09 | 0.68 |
| 32:QA:1492:A:O4' | 43:QL:47:LYS:NZ | 2.26 | 0.68 |
| 32:XA:64:G:H4' | 32:XA:65:U:H3' | 1.76 | 0.68 |
| 26:Y4:59:PHE:CE1 | 50:XS:64:GLU:HB2 | 2.28 | 0.68 |
| 1:YA:1073:A:H2' | 1:YA:1074:G:H8 | 1.59 | 0.68 |
| 1:RA:2749:A:H5' | 7:RH:3:ARG:HH21 | 1.58 | 0.68 |
| 6:RG:179:PRO:HB2 | 26:R4:42:PHE:CE2 | 2.25 | 0.68 |
| 1:YA:1028:A:N6 | 1:YA:1125:G:H2' | 2.09 | 0.68 |
| 1:YA:2785:C:OP1 | 4:YE:41:LYS:NZ | 2.25 | 0.68 |
| 32:XA:1285:A:H4' | 32:XA:1286:A:H5' | 1.76 | 0.68 |
| 41:XJ:35:SER:HB3 | 41:XJ:73:ASP:H | 1.59 | 0.68 |
| 1:YA:1073:A:H2' | 1:YA:1074:G:C8 | 2.28 | 0.68 |
| 55:XY:134:MET:HB2 | 55:XY:333:MET:HA | 1.76 | 0.67 |
| 32:QA:559:A:OP1 | 36:QE:126:ARG:NH2 | 2.26 | 0.67 |
| 44:XM:3:ARG:HG3 | 44:XM:8:GLU:HG3 | 1.76 | 0.67 |
| 1:YA:1798:U:H5' | 3:YD:259:THR:HG22 | 1.76 | 0.67 |
| 8:YI:50:ARG:O | 8:YI:54:GLN:NE2 | 2.27 | 0.67 |
| 33:QB:19:HIS:NE2 | 33:QB:189:ASP:OD2 | 2.27 | 0.67 |
| 21:RZ:45:ASP:OD1 | 21:RZ:49:ARG:NH1 | 2.27 | 0.67 |
| 1:YA:1087:G:H1 | 1:YA:1102:C:H42 | 1.41 | 0.67 |
| 37:QF:97:PHE:HB2 | 49:QR:32:ARG:HH11 | 1.60 | 0.67 |
| 32:XA:1183:A:O2' | 32:XA:1184:G:OP1 | 2.09 | 0.67 |
| 32:XA:474:G:H2' | 32:XA:475:G:H8 | 1.59 | 0.67 |
| 1:YA:1094:U:OP1 | 1:YA:1096:A:N6 | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:YG:41:GLN:HB3 | 6:YG:43:LEU:HD13 | 1.77 | 0.67 |
| 1:RA:1530:C:O2' | 1:RA:1531:C:O5' | 2.07 | 0.67 |
| 32:XA:316:G:OP2 | 32:XA:351:G:O2' | 2.13 | 0.67 |
| 1:RA:1310:G:OP2 | 29:R7:9:ARG:NH1 | 2.28 | 0.67 |
| 8:RI:109:ILE:HG13 | 8:RI:130:TYR:CZ | 2.30 | 0.67 |
| 32:XA:427:U:OP1 | 35:XD:13:ARG:NH2 | 2.28 | 0.67 |
| 36:XE:69:VAL:HG11 | 36:XE:113:ALA:HB1 | 1.74 | 0.67 |
| 6:YG:44:GLY:O | 6:YG:47:LYS:HD2 | 1.95 | 0.67 |
| 51:QT:57:ARG:HH12 | 51:QT:100:ILE:HD12 | 1.60 | 0.67 |
| 11:YP:59:LEU:HD21 | 30:Y8:10:ALA:HA | 1.77 | 0.67 |
| 33:XB:91:PRO:HG3 | 33:XB:155:LEU:HD23 | 1.77 | 0.66 |
| 1:YA:1266:G:O5' | 18:YW:15:ARG:NH2 | 2.28 | 0.66 |
| 20:YY:23:ARG:HG2 | 20:YY:42:VAL:HG22 | 1.77 | 0.66 |
| 6:RG:139:LEU:HD21 | 6:RG:149:VAL:HG11 | 1.75 | 0.66 |
| 55:XY:119:THR:N | 55:XY:302:ASP:OD2 | 2.28 | 0.66 |
| 1:YA:1049:C:H2' | 1:YA:1050:A:H8 | 1.60 | 0.66 |
| 1:YA:307:G:N1 | 1:YA:310:A:OP2 | 2.28 | 0.66 |
| 11:YP:2:LYS:NZ | 11:YP:4:SER:OG | 2.27 | 0.66 |
| 32:QA:78:G:H1 | 32:QA:91:C:N4 | 1.92 | 0.66 |
| 5:RF:165:ARG:HA | 5:RF:168:ARG:HD2 | 1.77 | 0.66 |
| 32:XA:1164:G:H1 | 32:XA:1172:C:H42 | 1.43 | 0.66 |
| 32:XA:976:G:H5' | 32:XA:1358:U:O2' | 1.95 | 0.66 |
| 34:XC:6:HIS:HD2 | 34:XC:9:GLY:H | 1.41 | 0.66 |
| 55:XY:186:ARG:HB3 | 55:XY:312:PHE:HD2 | 1.60 | 0.66 |
| 36:QE:79:GLU:HG3 | 36:QE:93:PRO:HD2 | 1.77 | 0.66 |
| 11:RP:52:GLU:OE1 | 11:RP:55:ARG:NH1 | 2.28 | 0.66 |
| 1:YA:2445:G:OP1 | 5:YF:74:ARG:NH2 | 2.22 | 0.66 |
| 1:RA:2751:G:C8 | 7:RH:2:SER:HA | 2.31 | 0.66 |
| 50:XS:41:VAL:HG12 | 50:XS:44:MET:HG3 | 1.76 | 0.66 |
| 32:QA:922:G:H4' | 36:QE:20:GLN:HA | 1.78 | 0.66 |
| 1:YA:1064:C:H3' | 1:YA:1065:U:H5' | 1.77 | 0.66 |
| 1:YA:987:G:O2' | 1:YA:1000:A:N3 | 2.29 | 0.66 |
| 43:XL:70:ILE:HG12 | 43:XL:100:ILE:HD12 | 1.78 | 0.66 |
| 4:YE:52:LEU:HB3 | 4:YE:53:PRO:HD2 | 1.76 | 0.66 |
| 1:RA:1923:U:OP1 | 53:QV:24:U:O2' | 2.14 | 0.66 |
| 1:RA:1064:C:H3' | 1:RA:1065:U:C5' | 2.26 | 0.66 |
| 32:XA:1318:A:H5" | 50:XS:3:ARG:HH22 | 1.61 | 0.66 |
| 1:YA:637:A:H8 | 11:YP:117:GLU:HG3 | 1.60 | 0.66 |
| 21:YZ:10:ARG:NH2 | 21:YZ:26:GLY:O | 2.28 | 0.66 |
| 27:R5:16:ARG:NH1 | 27:R5:17:ASP:OD1 | 2.29 | 0.65 |
| 32:QA:78:G:N2 | 32:QA:91:C:N3 | 2.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:QQ:66:SER:O | 48:QQ:70:ARG:NH1 | 2.29 | 0.65 |
| 1:RA:2218:U:O2 | 23:R1:52:ARG:NH2 | 2.29 | 0.65 |
| 32:XA:1136:U:OP2 | 32:XA:1137:C:N4 | 2.29 | 0.65 |
| 1:YA:2206:G:H5'' | 1:YA:2207:G:C8 | 2.30 | 0.65 |
| 4:YE:11:MET:HG2 | 4:YE:24:THR:HG22 | 1.77 | 0.65 |
| 35:QD:53:ASP:HB3 | 35:QD:57:ARG:HH12 | 1.60 | 0.65 |
| 1:RA:2785:C:OP1 | 4:RE:41:LYS:NZ | 2.30 | 0.65 |
| 12:RQ:21:THR:HG21 | 12:RQ:101:ARG:HB2 | 1.79 | 0.65 |
| 35:QD:173:TRP:CD2 | 35:QD:189:PRO:HG3 | 2.31 | 0.65 |
| 1:RA:2134:A:N6 | 1:RA:2156:G:O2' | 2.30 | 0.65 |
| 1:YA:857:C:OP2 | 22:Y0:77:ARG:NH2 | 2.30 | 0.65 |
| 23:Y1:75:GLU:HA | 23:Y1:78:LYS:HE2 | 1.78 | 0.65 |
| 1:YA:1064:C:H3' | 1:YA:1065:U:C5' | 2.25 | 0.65 |
| 51:QT:89:ARG:O | 51:QT:93:GLU:HG2 | 1.96 | 0.65 |
| 4:RE:111:ARG:HG3 | 4:RE:160:TYR:CD2 | 2.32 | 0.65 |
| 15:RT:55:ASN:N | 15:RT:59:THR:HG22 | 2.08 | 0.65 |
| 35:XD:175:SER:HB3 | 35:XD:186:LEU:HD11 | 1.78 | 0.65 |
| 1:YA:1031:G:O2' | 31:Y9:7:VAL:O | 2.12 | 0.65 |
| 42:XK:62:GLN:HB2 | 42:XK:93:GLN:HG3 | 1.79 | 0.65 |
| 1:YA:1693:U:O2' | 3:YD:14:ARG:NH2 | 2.30 | 0.65 |
| 32:QA:1030(D):G:N7 | 32:QA:1031:G:N2 | 2.44 | 0.65 |
| 32:XA:559:A:OP1 | 36:XE:126:ARG:NH2 | 2.29 | 0.65 |
| 1:YA:1028:A:H61 | 1:YA:1126:A:P | 2.19 | 0.65 |
| 1:YA:2128:C:N4 | 1:YA:2160:G:H1 | 1.90 | 0.65 |
| 12:YQ:34:LEU:HB2 | 12:YQ:118:LEU:HD22 | 1.77 | 0.65 |
| 35:QD:12:CYS:SG | 35:QD:19:LEU:HB2 | 2.37 | 0.65 |
| 35:XD:122:ARG:NH1 | 35:XD:134:ASP:O | 2.29 | 0.65 |
| 1:YA:2334:G:H5' | 14:YS:9:ARG:HG2 | 1.79 | 0.65 |
| 18:YW:14:PRO:HG2 | 18:YW:78:GLU:HG2 | 1.78 | 0.64 |
| 38:XG:113:GLU:HG2 | 38:XG:119:ARG:HG2 | 1.78 | 0.64 |
| 44:QM:3:ARG:HG3 | 44:QM:4:ILE:H | 1.63 | 0.64 |
| 32:XA:673:G:H2' | 32:XA:674:G:C8 | 2.32 | 0.64 |
| 1:RA:1064:C:H3' | 1:RA:1065:U:H5' | 1.78 | 0.64 |
| 36:XE:50:GLU:HB2 | 36:XE:53:LEU:HD13 | 1.80 | 0.64 |
| 1:YA:1049:C:H2' | 1:YA:1050:A:C8 | 2.33 | 0.64 |
| 1:YA:1786:A:H1' | 1:YA:1938:A:N6 | 2.12 | 0.64 |
| 32:QA:1086:U:H3 | 32:QA:1099:G:H22 | 1.45 | 0.64 |
| 40:X1:46:ALA:HB2 | 40:X1:74:ILE:HG23 | 1.79 | 0.64 |
| 1:YA:1029:A:C2 | 1:YA:2465:C:H2' | 2.32 | 0.64 |
| 1:YA:1385:G:O2' | 1:YA:1396:U:O2 | 2.15 | 0.64 |
| 1:YA:2128:C:N3 | 1:YA:2160:G:N2 | 2.45 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:RA:861:A:N3 | 2:RB:79:C:O2' | 2.30 | 0.64 |
| 23:Y1:76:ARG:HH22 | 23:Y1:97:LEU:HB3 | 1.62 | 0.64 |
| 26:Y4:58:ARG:NH1 | 50:XS:65:ASN:O | 2.30 | 0.64 |
| 21:YZ:19:ARG:NH1 | 21:YZ:84:GLU:O | 2.31 | 0.64 |
| 21:RZ:158:PRO:HG2 | 21:RZ:161:VAL:HG11 | 1.80 | 0.64 |
| 30:Y8:6:THR:HG22 | 30:Y8:63:PRO:HD2 | 1.78 | 0.64 |
| 32:QA:974:A:OP2 | 45:QN:29:ARG:NH2 | 2.30 | 0.64 |
| 1:RA:637:A:H8 | 11:RP:117:GLU:HG3 | 1.62 | 0.64 |
| 5:RF:157:VAL:HB | 5:RF:194:MET:HG2 | 1.79 | 0.64 |
| 32:XA:1004:A:H5' | 32:XA:1025:U:H5 | 1.63 | 0.64 |
| 1:YA:1065:U:H4' | 1:YA:1066:U:H5' | 1.80 | 0.64 |
| 1:YA:2156:G:N7 | 1:YA:2157:G:N2 | 2.46 | 0.64 |
| 8:YI:86:THR:HA | 8:YI:123:LEU:HD23 | 1.79 | 0.64 |
| 20:YY:102:CYS:SG | 20:YY:103:GLY:N | 2.71 | 0.64 |
| 1:RA:1053:C:H2' | 1:RA:1054:A:H8 | 1.62 | 0.64 |
| 1:RA:307:G:N1 | 1:RA:310:A:OP2 | 2.31 | 0.64 |
| 1:YA:2742:C:OP1 | 31:Y9:35:ARG:HD3 | 1.98 | 0.64 |
| 1:RA:1266:G:O5' | 18:RW:15:ARG:NH2 | 2.31 | 0.64 |
| 1:RA:309:G:N3 | 1:RA:329:G:O2' | 2.30 | 0.64 |
| 1:YA:143(A):G:H4' | 19:YX:35:THR:HG21 | 1.80 | 0.64 |
| 55:QY:183:ARG:HB3 | 55:QY:309:THR:HG22 | 1.80 | 0.63 |
| 1:RA:987:G:O2' | 1:RA:1000:A:N3 | 2.26 | 0.63 |
| 21:YZ:72:ARG:HG2 | 21:YZ:89:PHE:HB2 | 1.79 | 0.63 |
| 32:QA:269:C:H2' | 32:QA:270:A:C8 | 2.34 | 0.63 |
| 33:QB:96:ARG:HD2 | 33:QB:98:LEU:HD23 | 1.80 | 0.63 |
| 1:RA:11:G:H2' | 1:RA:12:U:H5' | 1.79 | 0.63 |
| 1:RA:2156:G:N7 | 1:RA:2157:G:N2 | 2.46 | 0.63 |
| 32:XA:1221:G:OP1 | 32:XA:1320:C:N4 | 2.28 | 0.63 |
| 1:YA:2464:C:H2' | 1:YA:2465:C:O4' | 1.98 | 0.63 |
| 6:YG:21:ARG:HE | 6:YG:22:ARG:HG2 | 1.63 | 0.63 |
| 1:RA:1028:A:N6 | 1:RA:1125:G:H2' | 2.13 | 0.63 |
| 1:YA:631:A:OP1 | 11:YP:65:ARG:NH1 | 2.30 | 0.63 |
| 1:RA:2327:A:H2' | 1:RA:2328:A:C8 | 2.34 | 0.63 |
| 1:RA:652(C):A:H61 | 1:RA:655:A:H1' | 1.64 | 0.63 |
| 40:XI:50:LEU:HD23 | 40:XI:85:LEU:HD11 | 1.80 | 0.63 |
| 26:Y4:48:ARG:HG3 | 26:Y4:52:THR:HG23 | 1.81 | 0.63 |
| 2:YB:24:G:N7 | 2:YB:56:G:H2' | 2.13 | 0.63 |
| 1:RA:1076:C:H4' | 1:RA:1077:A:OP1 | 1.97 | 0.63 |
| 10:RO:80:ASP:OD1 | 15:RT:64:ARG:NH2 | 2.32 | 0.63 |
| 1:YA:2206:G:H3' | 1:YA:2207:G:H8 | 1.63 | 0.63 |
| 32:XA:1288:A:O3' | 52:XU:10:ARG:NH2 | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:QF:25:ILE:HG13 | 37:QF:82:ARG:NH1 | 2.14 | 0.63 |
| 26:Y4:18:CYS:SG | 26:Y4:39:CYS:HB3 | 2.39 | 0.63 |
| 11:YP:126:VAL:HG12 | 11:YP:148:LEU:HD22 | 1.79 | 0.63 |
| 44:QM:15:VAL:HG11 | 44:QM:48:LEU:HD21 | 1.81 | 0.63 |
| 1:RA:2206:G:H3' | 1:RA:2207:G:C8 | 2.34 | 0.63 |
| 32:XA:1343:G:H4' | 40:XI:122:ALA:HB3 | 1.81 | 0.63 |
| 32:XA:581:G:OP1 | 46:XO:65:ARG:NH2 | 2.31 | 0.63 |
| 54:XX:19:U:N3 | 55:XY:121:GLY:O | 2.31 | 0.63 |
| 32:QA:73:G:H1 | 32:QA:96:U:H3 | 1.46 | 0.63 |
| 1:RA:1057:A:N7 | 1:RA:1086:A:H2' | 2.14 | 0.63 |
| 32:XA:1302:U:OP1 | 44:XM:13:LYS:NZ | 2.28 | 0.63 |
| 38:XG:15:ASP:OD1 | 38:XG:20:ASP:N | 2.31 | 0.63 |
| 1:YA:2126:A:H4' | 1:YA:2127:G:O5' | 1.98 | 0.62 |
| 32:QA:1519:MA6:O5' | 32:QA:1519:MA6:H8 | 1.99 | 0.62 |
| 38:QG:113:GLU:HG2 | 38:QG:119:ARG:HG2 | 1.80 | 0.62 |
| 1:RA:2744:G:N2 | 7:RH:143:GLN:OE1 | 2.30 | 0.62 |
| 32:QA:142:G:O2' | 32:QA:196:A:N1 | 2.33 | 0.62 |
| 1:RA:997:G:H5'' | 16:RU:92:ARG:HH21 | 1.63 | 0.62 |
| 55:XY:328:ARG:HH22 | 55:XY:339:MET:C | 2.02 | 0.62 |
| 1:YA:2552:2MU:C6 | 1:YA:2552:2MU:C4 | 2.55 | 0.62 |
| 14:YS:15:ARG:O | 14:YS:19:LYS:HG2 | 1.98 | 0.62 |
| 32:QA:1075:C:OP1 | 33:QB:179:LYS:NZ | 2.31 | 0.62 |
| 32:XA:1187:G:OP1 | 40:XI:113:LYS:NZ | 2.32 | 0.62 |
| 1:YA:2206:G:H3' | 1:YA:2207:G:C8 | 2.33 | 0.62 |
| 36:QE:143:ARG:NH1 | 39:QH:77:GLU:OE2 | 2.32 | 0.62 |
| 23:R1:50:ARG:HG2 | 23:R1:59:THR:HG22 | 1.81 | 0.62 |
| 1:RA:1063:G:N2 | 1:RA:1075:C:N3 | 2.48 | 0.62 |
| 1:RA:2646:C:OP2 | 1:RA:2732:G:O2' | 2.17 | 0.62 |
| 32:XA:1128:C:H1' | 32:XA:1147:C:H42 | 1.65 | 0.62 |
| 35:QD:108:LEU:HD22 | 35:QD:174:LEU:HD13 | 1.82 | 0.62 |
| 55:QY:219:PRO:O | 55:QY:222:LEU:N | 2.30 | 0.62 |
| 36:QE:8:GLU:OE2 | 36:QE:63:ARG:NH2 | 2.32 | 0.62 |
| 1:YA:1379:A:H4' | 1:YA:1380:G:OP2 | 2.00 | 0.62 |
| 1:YA:483:A:O2' | 20:YY:49:VAL:O | 2.15 | 0.62 |
| 41:QJ:52:GLY:O | 45:QN:41:ARG:NH2 | 2.33 | 0.62 |
| 51:QT:60:GLU:HG3 | 51:QT:81:LYS:HD2 | 1.81 | 0.62 |
| 33:XB:77:ALA:HB2 | 33:XB:211:ILE:HD13 | 1.82 | 0.62 |
| 36:XE:102:ALA:HB1 | 36:XE:106:PRO:HG2 | 1.81 | 0.62 |
| 3:YD:108:PRO:HB3 | 3:YD:143:HIS:CE1 | 2.35 | 0.62 |
| 17:YV:62:LEU:HD21 | 17:YV:95:LEU:HB2 | 1.81 | 0.62 |
| 32:QA:976:G:H5' | 32:QA:1358:U:O2' | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:RP:63:PRO:HG2 | 30:R8:25:MET:HB2 | 1.80 | 0.61 |
| 32:XA:1494:G:O3' | 55:XY:160:LYS:NZ | 2.26 | 0.61 |
| 32:QA:1020:U:H2' | 32:QA:1021:G:C8 | 2.35 | 0.61 |
| 53:QV:1:C:H42 | 53:QV:72:A:H61 | 1.48 | 0.61 |
| 6:RG:108:ASN:O | 26:R4:37:SER:N | 2.33 | 0.61 |
| 1:RA:2839:G:H5' | 13:RR:46:GLY:HA2 | 1.81 | 0.61 |
| 53:XV:4:G:HO2' | 53:XV:5:G:H8 | 1.48 | 0.61 |
| 36:QE:8:GLU:HG2 | 36:QE:34:VAL:HG22 | 1.80 | 0.61 |
| 55:QY:316:ARG:NE | 55:QY:327:TYR:OH | 2.33 | 0.61 |
| 1:RA:1530:C:H42 | 1:RA:1539:G:H1 | 1.47 | 0.61 |
| 32:XA:865:A:H5' | 32:XA:1078:U:C5 | 2.35 | 0.61 |
| 32:XA:437:U:H5' | 35:XD:155:LEU:HD21 | 1.82 | 0.61 |
| 32:QA:1003:G:H2' | 32:QA:1004:A:H4' | 1.81 | 0.61 |
| 33:QB:21:ARG:O | 33:QB:23:ARG:N | 2.29 | 0.61 |
| 40:XI:50:LEU:HB2 | 40:XI:56:LEU:HD23 | 1.82 | 0.61 |
| 37:QF:10:LEU:HD21 | 37:QF:61:LEU:HD22 | 1.81 | 0.61 |
| 1:RA:2126:A:H4' | 1:RA:2127:G:O5' | 2.01 | 0.61 |
| 44:XM:96:LEU:O | 44:XM:110:ARG:NH1 | 2.34 | 0.61 |
| 1:YA:2122:U:H3 | 1:YA:2176:A:H61 | 1.48 | 0.61 |
| 44:QM:13:LYS:HA | 44:QM:44:ARG:HH11 | 1.64 | 0.61 |
| 1:RA:1057:A:O2' | 1:RA:1058:G:OP1 | 2.18 | 0.61 |
| 1:RA:2206:G:H5'' | 1:RA:2207:G:C8 | 2.36 | 0.61 |
| 1:RA:272(L):U:H5' | 8:RI:50:ARG:HH12 | 1.64 | 0.61 |
| 32:XA:1025:U:H3 | 32:XA:1036:G:H1 | 1.48 | 0.61 |
| 26:Y4:59:PHE:CA | 26:Y4:61:ARG:H | 2.10 | 0.61 |
| 39:QH:64:LYS:HG2 | 39:QH:79:VAL:HG21 | 1.83 | 0.61 |
| 1:RA:998:C:P | 16:RU:92:ARG:HH22 | 2.23 | 0.61 |
| 33:XB:76:GLN:HB2 | 33:XB:208:ILE:HG12 | 1.83 | 0.61 |
| 1:YA:1063:G:N2 | 1:YA:1075:C:N3 | 2.48 | 0.61 |
| 1:YA:2839:G:H5' | 13:YR:46:GLY:HA2 | 1.83 | 0.61 |
| 32:QA:297:G:N2 | 32:QA:300:A:OP2 | 2.30 | 0.61 |
| 1:RA:1067:A:H4' | 1:RA:1068:G:OP2 | 2.01 | 0.61 |
| 32:XA:1073:U:O2' | 33:XB:104:ASN:OD1 | 2.19 | 0.61 |
| 33:XB:101:MET:HA | 33:XB:108:ILE:HG13 | 1.83 | 0.61 |
| 1:YA:11:G:H2' | 1:YA:12:U:H5' | 1.83 | 0.61 |
| 1:YA:652(U):C:H2' | 1:YA:652(V):G:C8 | 2.36 | 0.61 |
| 33:QB:69:LEU:HD13 | 33:QB:91:PRO:HB2 | 1.83 | 0.61 |
| 1:RA:2128:C:N3 | 1:RA:2160:G:N2 | 2.42 | 0.61 |
| 32:XA:102:G:O2' | 32:XA:151:A:N3 | 2.30 | 0.61 |
| 1:YA:1423:G:OP1 | 1:YA:1492:G:O2' | 2.19 | 0.61 |
| 33:QB:195:ASP:O | 39:QH:68:ARG:NH2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:RA:1379:A:H4' | 1:RA:1380:G:OP2 | 2.00 | 0.60 |
| 1:RA:2612:C:OP2 | 27:R5:2:ALA:N | 2.34 | 0.60 |
| 34:XC:152:ILE:HG13 | 34:XC:199:LYS:HB2 | 1.81 | 0.60 |
| 25:Y3:8:LEU:HD12 | 25:Y3:31:LEU:HA | 1.83 | 0.60 |
| 26:Y4:16:CYS:SG | 26:Y4:17:GLY:N | 2.74 | 0.60 |
| 1:YA:1639:U:H2' | 1:YA:1640:C:H5'' | 1.83 | 0.60 |
| 32:QA:791:G:N2 | 32:QA:1497:G:O3' | 2.34 | 0.60 |
| 34:QC:6:HIS:CE1 | 34:QC:8:ILE:HB | 2.35 | 0.60 |
| 35:QD:88:VAL:HG22 | 36:QE:96:PRO:HB2 | 1.83 | 0.60 |
| 1:RA:2206:G:H3' | 1:RA:2207:G:H8 | 1.65 | 0.60 |
| 1:RA:2286:A:C8 | 28:R6:34:LEU:HD21 | 2.36 | 0.60 |
| 5:RF:185:ASP:HA | 5:RF:188:ARG:HD3 | 1.84 | 0.60 |
| 32:XA:266:G:O3' | 48:XQ:67:LYS:HB2 | 2.00 | 0.60 |
| 1:YA:1050:A:C2 | 1:YA:2751:G:C2 | 2.89 | 0.60 |
| 1:YA:334:C:OP1 | 1:YA:335:C:N4 | 2.34 | 0.60 |
| 1:YA:2306:C:N4 | 6:YG:43:LEU:O | 2.33 | 0.60 |
| 36:QE:33:VAL:HG21 | 36:QE:109:ILE:HA | 1.82 | 0.60 |
| 41:QJ:11:PHE:HE1 | 41:QJ:67:THR:HG22 | 1.65 | 0.60 |
| 55:QY:263:GLN:O | 55:QY:267:LYS:N | 2.33 | 0.60 |
| 21:YZ:144:LEU:HD21 | 21:YZ:150:LEU:HD13 | 1.83 | 0.60 |
| 15:RT:95:ARG:HG2 | 15:RT:95:ARG:HH11 | 1.65 | 0.60 |
| 20:RY:102:CYS:SG | 20:RY:103:GLY:N | 2.74 | 0.60 |
| 32:XA:1002:G:H2' | 32:XA:1003:G:C8 | 2.36 | 0.60 |
| 32:XA:1319:A:OP2 | 50:XS:3:ARG:NH2 | 2.32 | 0.60 |
| 26:Y4:61:ARG:NH2 | 50:XS:9:VAL:HG11 | 2.16 | 0.60 |
| 1:YA:784:A:C6 | 3:YD:229:VAL:HG11 | 2.36 | 0.60 |
| 32:QA:921:U:O2 | 36:QE:19:MET:HB2 | 2.01 | 0.60 |
| 23:R1:51:VAL:HG11 | 23:R1:74:VAL:HG21 | 1.84 | 0.60 |
| 1:RA:2122:U:H3 | 1:RA:2176:A:H61 | 1.50 | 0.60 |
| 28:Y6:13:CYS:SG | 28:Y6:47:THR:HG21 | 2.42 | 0.60 |
| 32:QA:612:C:O2 | 32:QA:629:G:N2 | 2.35 | 0.60 |
| 46:QO:39:LEU:HD13 | 46:QO:56:LEU:HB2 | 1.82 | 0.60 |
| 15:RT:24:PRO:HA | 15:RT:49:VAL:HG23 | 1.84 | 0.60 |
| 1:YA:1038:C:N4 | 1:YA:1117:G:H1 | 1.98 | 0.60 |
| 38:QG:27:ILE:HD12 | 38:QG:40:ALA:HA | 1.82 | 0.60 |
| 1:RA:1507:A:O2' | 1:RA:1508:A:O5' | 2.18 | 0.60 |
| 33:XB:16:HIS:CG | 33:XB:210:SER:HB3 | 2.37 | 0.60 |
| 1:YA:2261:C:OP1 | 22:Y0:19:LYS:NZ | 2.29 | 0.60 |
| 2:YB:13:A:N1 | 2:YB:69:G:O2' | 2.28 | 0.60 |
| 32:QA:1070:U:OP1 | 36:QE:20:GLN:NE2 | 2.24 | 0.60 |
| 32:QA:901:A:O2' | 32:QA:1513:A:OP1 | 2.11 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:RP:59:LEU:HD21 | 30:R8:10:ALA:HA | 1.83 | 0.60 |
| 9:RN:15:LEU:HB2 | 9:RN:135:PRO:HB2 | 1.83 | 0.60 |
| 41:XJ:11:PHE:HE1 | 41:XJ:67:THR:HG22 | 1.65 | 0.60 |
| 35:QD:162:LEU:HD13 | 35:QD:181:MET:HG2 | 1.84 | 0.60 |
| 32:XA:769:G:H4' | 32:XA:1513:A:H4' | 1.84 | 0.60 |
| 33:XB:187:LEU:HA | 33:XB:201:ILE:HB | 1.83 | 0.60 |
| 1:RA:1798:U:OP2 | 3:RD:274:ARG:NH2 | 2.31 | 0.59 |
| 32:XA:696:A:N1 | 32:XA:797:C:O2' | 2.30 | 0.59 |
| 1:YA:2527:C:O4' | 31:Y9:1:MET:N | 2.35 | 0.59 |
| 4:YE:12:THR:HG22 | 4:YE:13:ARG:H | 1.66 | 0.59 |
| 32:QA:335:C:H1' | 32:QA:1434:A:H1' | 1.84 | 0.59 |
| 32:QA:955:U:OP1 | 55:QY:137:ARG:NH1 | 2.34 | 0.59 |
| 32:QA:1298:C:C4 | 38:QG:114:ARG:HD2 | 2.37 | 0.59 |
| 39:QH:51:VAL:HG12 | 39:QH:52:ASP:H | 1.67 | 0.59 |
| 32:XA:1360:A:OP2 | 45:XN:35:ARG:NH2 | 2.36 | 0.59 |
| 55:XY:326:LEU:HD21 | 55:XY:328:ARG:HH21 | 1.66 | 0.59 |
| 22:Y0:27:GLU:HG3 | 22:Y0:68:GLU:HA | 1.84 | 0.59 |
| 1:YA:674:G:H1' | 5:YF:74:ARG:HD3 | 1.84 | 0.59 |
| 32:QA:1010:G:N2 | 32:QA:1020:U:H1' | 2.17 | 0.59 |
| 32:QA:642:A:N3 | 39:QH:113:SER:OG | 2.33 | 0.59 |
| 55:QY:263:GLN:HA | 55:QY:266:ASN:HB2 | 1.83 | 0.59 |
| 8:RI:69:LYS:NZ | 8:RI:137:PRO:O | 2.27 | 0.59 |
| 33:XB:118:LEU:HD13 | 33:XB:142:LEU:HB2 | 1.84 | 0.59 |
| 9:YN:15:LEU:HB2 | 9:YN:135:PRO:HB2 | 1.84 | 0.59 |
| 32:QA:1435:G:H2' | 32:QA:1436:U:C6 | 2.36 | 0.59 |
| 36:QE:57:LYS:HG2 | 36:QE:61:TYR:CE2 | 2.37 | 0.59 |
| 1:RA:2749:A:H5' | 7:RH:3:ARG:NH2 | 2.17 | 0.59 |
| 1:RA:2748:A:H5' | 7:RH:4:ILE:HD12 | 1.84 | 0.59 |
| 33:XB:8:LYS:HG2 | 33:XB:9:GLU:H | 1.68 | 0.59 |
| 1:YA:1800:C:OP2 | 3:YD:183:ARG:NH2 | 2.35 | 0.59 |
| 3:YD:71:ASP:HB3 | 3:YD:103:ARG:HH22 | 1.67 | 0.59 |
| 6:YG:80:PHE:O | 6:YG:82:LEU:N | 2.35 | 0.59 |
| 1:RA:674:G:H1' | 5:RF:74:ARG:HD3 | 1.83 | 0.59 |
| 1:YA:1530:C:H42 | 1:YA:1539:G:H1 | 1.50 | 0.59 |
| 1:YA:2787:C:H1' | 4:YE:62:PRO:HG3 | 1.84 | 0.59 |
| 6:YG:77:ILE:HG21 | 6:YG:80:PHE:CD2 | 2.36 | 0.59 |
| 32:QA:17:U:H2' | 32:QA:18:C:C6 | 2.37 | 0.59 |
| 32:QA:256:U:OP1 | 48:QQ:17:LYS:NZ | 2.30 | 0.59 |
| 1:RA:1639:U:H2' | 1:RA:1640:C:H5'' | 1.83 | 0.59 |
| 1:RA:270:A:OP2 | 1:RA:272(X):G:N1 | 2.29 | 0.59 |
| 51:XT:50:GLU:HG3 | 51:XT:100:ILE:HD11 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:2279:G:N7 | 22:Y0:14:ARG:NH1 | 2.50 | 0.59 |
| 37:QF:99:ALA:HB2 | 49:QR:31:LEU:HD21 | 1.83 | 0.59 |
| 55:QY:217:ILE:HD12 | 55:QY:274:LEU:HD12 | 1.84 | 0.59 |
| 1:RA:2150:U:H2' | 1:RA:2151:G:C8 | 2.37 | 0.59 |
| 7:RH:11:VAL:HG21 | 7:RH:50:VAL:HG23 | 1.85 | 0.59 |
| 23:Y1:50:ARG:HG2 | 23:Y1:59:THR:HG22 | 1.84 | 0.59 |
| 32:QA:673:G:H2' | 32:QA:674:G:C8 | 2.38 | 0.59 |
| 36:QE:137:GLU:OE1 | 36:QE:141:GLN:NE2 | 2.29 | 0.59 |
| 1:YA:1076:C:H4' | 1:YA:1077:A:OP1 | 2.02 | 0.59 |
| 34:QC:8:ILE:HG23 | 34:QC:16:ARG:HG2 | 1.84 | 0.59 |
| 36:QE:74:GLY:HA3 | 36:QE:116:THR:HG22 | 1.85 | 0.59 |
| 23:R1:3:LYS:HG3 | 23:R1:4:VAL:H | 1.68 | 0.59 |
| 1:RA:2001:A:H2' | 1:RA:2002:G:C8 | 2.38 | 0.59 |
| 32:XA:1376:U:H2' | 32:XA:1377:A:H8 | 1.67 | 0.59 |
| 32:XA:17:U:H2' | 32:XA:18:C:C6 | 2.38 | 0.59 |
| 36:XE:12:LEU:HD12 | 36:XE:128:PRO:HB2 | 1.85 | 0.59 |
| 32:QA:1256:A:OP2 | 32:QA:1279:A:N6 | 2.36 | 0.59 |
| 1:RA:2304:G:H22 | 1:RA:2312:U:H3 | 1.48 | 0.59 |
| 39:XH:10:LEU:HD22 | 39:XH:83:ILE:HD11 | 1.84 | 0.59 |
| 1:YA:1507:A:O2' | 1:YA:1508:A:O5' | 2.19 | 0.59 |
| 1:YA:588:U:H2' | 1:YA:589:C:C6 | 2.38 | 0.59 |
| 3:YD:206:LEU:HD22 | 3:YD:211:ARG:HG2 | 1.85 | 0.59 |
| 35:QD:106:TYR:HE2 | 35:QD:107:ARG:HH11 | 1.50 | 0.58 |
| 17:RV:72:VAL:HG13 | 17:RV:85:LYS:HB3 | 1.84 | 0.58 |
| 32:XA:1129:C:H2' | 32:XA:1139:G:N7 | 2.17 | 0.58 |
| 37:XF:10:LEU:HD21 | 37:XF:61:LEU:HD22 | 1.84 | 0.58 |
| 2:YB:91:C:OP2 | 12:YQ:16:ARG:NH1 | 2.36 | 0.58 |
| 33:QB:167:PRO:HG3 | 33:QB:186:ALA:HB1 | 1.85 | 0.58 |
| 33:QB:54:THR:HG21 | 33:QB:201:ILE:HD11 | 1.85 | 0.58 |
| 14:RS:59:LYS:HD2 | 14:RS:60:GLY:N | 2.12 | 0.58 |
| 32:XA:890:G:O2' | 32:XA:906:G:O6 | 2.18 | 0.58 |
| 1:YA:652(C):A:H61 | 1:YA:655:A:H1' | 1.68 | 0.58 |
| 5:YF:178:PRO:HB2 | 5:YF:201:VAL:CG2 | 2.31 | 0.58 |
| 7:YH:113:VAL:HG11 | 7:YH:151:ILE:HD13 | 1.84 | 0.58 |
| 11:YP:86:LYS:HB3 | 11:YP:118:GLY:HA3 | 1.85 | 0.58 |
| 34:QC:6:HIS:HE1 | 34:QC:8:ILE:HB | 1.69 | 0.58 |
| 35:QD:170:VAL:HG12 | 35:QD:174:LEU:HB2 | 1.84 | 0.58 |
| 36:XE:74:GLY:HA3 | 36:XE:116:THR:HG22 | 1.85 | 0.58 |
| 31:Y9:25:VAL:HB | 31:Y9:34:GLN:HB2 | 1.85 | 0.58 |
| 1:YA:878:A:H3' | 1:YA:879:G:H8 | 1.68 | 0.58 |
| 4:YE:24:THR:HG23 | 4:YE:186:GLY:O | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:YF:11:VAL:HB | 5:YF:18:ARG:HB3 | 1.85 | 0.58 |
| 21:YZ:5:LEU:HD11 | 21:YZ:39:VAL:HB | 1.84 | 0.58 |
| 32:QA:677:U:H3 | 32:QA:713:G:H22 | 1.52 | 0.58 |
| 43:QL:70:ILE:HG12 | 43:QL:100:ILE:HD12 | 1.86 | 0.58 |
| 4:RE:119:ARG:HD3 | 4:RE:160:TYR:HB2 | 1.85 | 0.58 |
| 32:QA:441:A:H3' | 32:QA:442:C:H6 | 1.69 | 0.58 |
| 1:RA:652(U):C:H2' | 1:RA:652(V):G:C8 | 2.37 | 0.58 |
| 1:RA:2747:G:OP1 | 7:RH:138:LYS:NZ | 2.34 | 0.58 |
| 1:YA:1721:G:H2' | 1:YA:1740:G:O6 | 2.04 | 0.58 |
| 1:YA:2218:U:O2 | 23:Y1:52:ARG:NH2 | 2.36 | 0.58 |
| 1:YA:2347:C:OP1 | 28:Y6:38:LYS:NZ | 2.25 | 0.58 |
| 1:YA:301:G:OP2 | 20:YY:84:ARG:NH2 | 2.37 | 0.58 |
| 36:QE:92:LYS:HB3 | 36:QE:119:LEU:HB2 | 1.86 | 0.58 |
| 53:QV:28:C:H2' | 53:QV:29:G:C8 | 2.39 | 0.58 |
| 7:YH:11:VAL:HG21 | 7:YH:50:VAL:HG23 | 1.85 | 0.58 |
| 32:QA:1292:U:OP2 | 38:QG:41:ARG:NH2 | 2.37 | 0.58 |
| 55:QY:262:SER:HB3 | 55:QY:265:LYS:HG2 | 1.84 | 0.58 |
| 32:XA:164:U:H2' | 32:XA:165:C:C6 | 2.39 | 0.58 |
| 1:YA:2502:G:H5'' | 1:YA:2503:2MA:H5'' | 1.84 | 0.58 |
| 10:YO:115:VAL:HG13 | 10:YO:121:VAL:HG21 | 1.85 | 0.58 |
| 19:YX:11:PRO:HB3 | 19:YX:92:LEU:HD11 | 1.86 | 0.58 |
| 32:QA:1375:A:H4' | 38:QG:29:LYS:HE2 | 1.85 | 0.58 |
| 3:YD:182:LEU:HB2 | 3:YD:272:ALA:HB3 | 1.85 | 0.58 |
| 32:QA:45:U:H2' | 32:QA:46:G:C8 | 2.38 | 0.58 |
| 55:QY:182:HIS:HB3 | 55:QY:310:TYR:HE1 | 1.69 | 0.58 |
| 6:RG:115:ARG:HB3 | 6:RG:136:ARG:HH22 | 1.69 | 0.58 |
| 34:XC:6:HIS:CD2 | 34:XC:9:GLY:H | 2.22 | 0.58 |
| 1:YA:2573:C:N4 | 55:XY:228:ARG:HE | 2.02 | 0.58 |
| 1:YA:2110:G:H5'' | 1:YA:2111:C:H5 | 1.69 | 0.58 |
| 1:YA:2150:U:H2' | 1:YA:2151:G:C8 | 2.38 | 0.58 |
| 32:QA:1441:G:O2' | 32:QA:1460:A:N6 | 2.36 | 0.57 |
| 32:QA:992:U:H4' | 32:QA:993:G:H5' | 1.86 | 0.57 |
| 37:QF:69:GLU:O | 37:QF:72:VAL:HG12 | 2.04 | 0.57 |
| 7:RH:40:GLU:OE1 | 7:RH:60:ARG:NH1 | 2.36 | 0.57 |
| 32:XA:1004:A:N7 | 32:XA:1037:C:H2' | 2.18 | 0.57 |
| 32:XA:473:G:OP2 | 47:XP:75:ARG:HD3 | 2.04 | 0.57 |
| 32:XA:933:G:O6 | 38:XG:3:ARG:NH2 | 2.35 | 0.57 |
| 1:YA:1056:G:N1 | 1:YA:1102:C:OP2 | 2.37 | 0.57 |
| 32:QA:222:U:H2' | 32:QA:223:U:C6 | 2.39 | 0.57 |
| 49:QR:32:ARG:HA | 49:QR:69:THR:HG21 | 1.86 | 0.57 |
| 40:XI:9:ARG:HG2 | 40:XI:14:VAL:HG12 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:XY:263:GLN:HA | 55:XY:266:ASN:HB2 | 1.86 | 0.57 |
| 1:YA:1053:C:H2' | 1:YA:1054:A:H8 | 1.68 | 0.57 |
| 1:YA:1087:G:N2 | 1:YA:1102:C:N3 | 2.43 | 0.57 |
| 33:QB:115:LEU:O | 33:QB:119:GLU:HG2 | 2.03 | 0.57 |
| 1:RA:2529:G:O6 | 31:R9:31:LYS:NZ | 2.37 | 0.57 |
| 32:XA:1412:C:H2' | 32:XA:1413:A:C8 | 2.39 | 0.57 |
| 34:XC:179:ARG:NH1 | 34:XC:206:GLU:OE1 | 2.35 | 0.57 |
| 46:XO:25:THR:HG21 | 46:XO:70:LEU:HB2 | 1.86 | 0.57 |
| 55:XY:200:ALA:HB3 | 55:XY:302:ASP:CB | 2.32 | 0.57 |
| 1:YA:2115:G:N1 | 1:YA:2119:A:OP2 | 2.38 | 0.57 |
| 1:YA:2152:G:H2' | 1:YA:2153:G:C8 | 2.40 | 0.57 |
| 1:YA:1049:C:N4 | 1:YA:2751:G:O6 | 2.33 | 0.57 |
| 32:QA:737:A:H2' | 32:QA:738:C:C6 | 2.39 | 0.57 |
| 1:RA:1087:G:H1 | 1:RA:1102:C:N4 | 2.02 | 0.57 |
| 1:RA:247:G:H4' | 1:RA:386:G:C5 | 2.40 | 0.57 |
| 5:RF:184:TYR:CE2 | 5:RF:188:ARG:HD2 | 2.40 | 0.57 |
| 32:QA:1013:G:N2 | 32:QA:1016:A:OP2 | 2.35 | 0.57 |
| 32:QA:159:G:N2 | 32:QA:161:A:H3' | 2.20 | 0.57 |
| 33:QB:178:ARG:HH22 | 39:QH:68:ARG:HH12 | 1.53 | 0.57 |
| 1:RA:1889:A:N1 | 1:RA:2234:G:H1' | 2.19 | 0.57 |
| 7:RH:3:ARG:HD3 | 7:RH:54:ARG:HH12 | 1.70 | 0.57 |
| 32:XA:1191:A:OP2 | 34:XC:3:ASN:ND2 | 2.37 | 0.57 |
| 32:XA:662:G:H2' | 32:XA:663:A:C8 | 2.40 | 0.57 |
| 33:QB:229:VAL:HG12 | 33:QB:230:VAL:H | 1.68 | 0.57 |
| 35:QD:166:LYS:N | 35:QD:168:ARG:HH21 | 2.02 | 0.57 |
| 1:RA:2127:G:H2' | 1:RA:2128:C:O4' | 2.04 | 0.57 |
| 7:RH:3:ARG:HB3 | 7:RH:6:ARG:HG2 | 1.87 | 0.57 |
| 32:XA:1023:G:H3' | 32:XA:1024:G:H8 | 1.70 | 0.57 |
| 34:XC:40:ARG:NH2 | 34:XC:55:VAL:O | 2.38 | 0.57 |
| 1:YA:2115:G:H21 | 1:YA:2171:A:H61 | 1.53 | 0.57 |
| 32:QA:1286:A:H2' | 32:QA:1287:A:H4' | 1.87 | 0.57 |
| 33:QB:16:HIS:HB2 | 33:QB:204:ASN:HB3 | 1.87 | 0.57 |
| 38:QG:89:MET:HE1 | 38:QG:155:ARG:HB2 | 1.87 | 0.57 |
| 1:RA:1786:A:H1' | 1:RA:1938:A:N6 | 2.19 | 0.57 |
| 32:XA:1435:G:H2' | 32:XA:1436:U:C6 | 2.40 | 0.57 |
| 32:XA:474:G:H2' | 32:XA:475:G:C8 | 2.40 | 0.57 |
| 1:YA:1371:G:HO2' | 1:YA:1372:U:H5 | 1.53 | 0.57 |
| 32:QA:1179:A:OP2 | 40:QI:93:ARG:NH2 | 2.38 | 0.57 |
| 32:QA:539:A:OP2 | 43:QL:115:LYS:NZ | 2.38 | 0.57 |
| 1:RA:2115:G:N1 | 1:RA:2119:A:OP2 | 2.38 | 0.57 |
| 1:RA:992:C:OP1 | 16:RU:47:TYR:OH | 2.14 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:RD:71:ASP:HB3 | 3:RD:103:ARG:NH2 | 2.19 | 0.57 |
| 4:RE:2:LYS:HB2 | 4:RE:95:ILE:HD12 | 1.86 | 0.57 |
| 5:RF:51:THR:HB | 5:RF:88:VAL:HG11 | 1.86 | 0.57 |
| 33:XB:7:VAL:O | 33:XB:217:ARG:NE | 2.32 | 0.57 |
| 32:XA:953:G:N7 | 44:XM:104:ARG:NH2 | 2.52 | 0.57 |
| 1:YA:1688:U:O2 | 1:YA:1700:A:H5' | 2.05 | 0.57 |
| 32:QA:1216:G:H5'' | 45:QN:5:ALA:HB2 | 1.84 | 0.56 |
| 5:RF:64:ILE:HG21 | 5:RF:78:ILE:HG23 | 1.87 | 0.56 |
| 13:RR:83:ILE:O | 13:RR:86:ARG:HG2 | 2.04 | 0.56 |
| 33:XB:229:VAL:HG12 | 33:XB:230:VAL:H | 1.68 | 0.56 |
| 36:XE:137:GLU:HG2 | 36:XE:140:ARG:HH11 | 1.69 | 0.56 |
| 32:XA:921:U:O2 | 36:XE:19:MET:HB2 | 2.05 | 0.56 |
| 43:XL:60:LEU:HD21 | 43:XL:66:VAL:HG22 | 1.87 | 0.56 |
| 1:RA:1049:C:H2' | 1:RA:1050:A:H8 | 1.70 | 0.56 |
| 7:RH:90:LYS:HD3 | 7:RH:159:GLU:HG2 | 1.87 | 0.56 |
| 32:XA:35:G:O2' | 43:XL:118:SER:O | 2.21 | 0.56 |
| 1:YA:1057:A:O2' | 1:YA:1058:G:OP1 | 2.19 | 0.56 |
| 1:YA:1086:A:OP1 | 1:YA:1104:C:O2' | 2.23 | 0.56 |
| 7:YH:40:GLU:OE1 | 7:YH:60:ARG:NH1 | 2.38 | 0.56 |
| 33:QB:185:ILE:HG22 | 33:QB:199:TYR:HB2 | 1.86 | 0.56 |
| 1:RA:876:C:H2' | 1:RA:877:U:O4' | 2.05 | 0.56 |
| 1:YA:2321:G:O2' | 1:YA:2322:A:OP1 | 2.21 | 0.56 |
| 1:YA:637:A:H5'' | 11:YP:117:GLU:HG2 | 1.87 | 0.56 |
| 55:QY:332:VAL:HG13 | 55:QY:337:LEU:HB3 | 1.88 | 0.56 |
| 1:YA:796:C:H2' | 1:YA:797:C:C6 | 2.40 | 0.56 |
| 1:YA:2012:G:OP1 | 18:YW:11:ARG:NH2 | 2.38 | 0.56 |
| 19:RX:35:THR:HG22 | 19:RX:37:THR:H | 1.70 | 0.56 |
| 21:RZ:19:ARG:NH1 | 21:RZ:84:GLU:O | 2.38 | 0.56 |
| 32:XA:919:A:O2' | 32:XA:1080:A:N1 | 2.26 | 0.56 |
| 32:XA:38:G:H22 | 32:XA:397:A:H5'' | 1.69 | 0.56 |
| 34:XC:57:ILE:HG12 | 34:XC:66:VAL:HG22 | 1.88 | 0.56 |
| 1:YA:714:U:N3 | 1:YA:717:G:OP2 | 2.24 | 0.56 |
| 32:QA:1030(A):C:N4 | 32:QA:1032:G:O6 | 2.38 | 0.56 |
| 32:QA:966:M2G:HM12 | 53:QV:34:C:H5' | 1.86 | 0.56 |
| 33:QB:27:LYS:HD2 | 33:QB:193:ASP:OD1 | 2.06 | 0.56 |
| 24:R2:23:LYS:O | 24:R2:27:GLU:HG3 | 2.05 | 0.56 |
| 32:XA:1305:G:N2 | 32:XA:1331:G:H1' | 2.20 | 0.56 |
| 32:XA:539:A:H2' | 32:XA:540:G:C8 | 2.41 | 0.56 |
| 33:XB:88:ALA:HB2 | 33:XB:219:VAL:HG13 | 1.87 | 0.56 |
| 55:XY:228:ARG:HA | 55:XY:241:ASP:HA | 1.86 | 0.56 |
| 1:YA:300:A:O2' | 1:YA:318:C:O2 | 2.22 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:YR:18:LEU:HD11 | 13:YR:22:ARG:CZ | 2.35 | 0.56 |
| 17:YV:35:LEU:HB2 | 17:YV:57:VAL:HG22 | 1.88 | 0.56 |
| 33:QB:16:HIS:HB3 | 33:QB:210:SER:HB2 | 1.87 | 0.56 |
| 53:QV:52:G:N3 | 53:QV:52:G:H2' | 2.21 | 0.56 |
| 1:RA:517:C:OP1 | 27:R5:16:ARG:NH2 | 2.39 | 0.56 |
| 9:RN:120:LEU:HD22 | 9:RN:122:VAL:HG23 | 1.88 | 0.56 |
| 15:RT:64:ARG:HB2 | 15:RT:73:GLU:HG2 | 1.87 | 0.56 |
| 35:XD:12:CYS:SG | 35:XD:19:LEU:HB2 | 2.46 | 0.56 |
| 1:YA:876:C:H2' | 1:YA:877:U:O4' | 2.06 | 0.56 |
| 5:RF:29:ASN:HB3 | 5:RF:112:MET:HE1 | 1.87 | 0.56 |
| 32:XA:1353:G:OP1 | 52:XU:10:ARG:NH1 | 2.39 | 0.56 |
| 55:XY:114:GLU:HB3 | 55:XY:163:ILE:HB | 1.87 | 0.56 |
| 46:QO:11:VAL:HG21 | 46:QO:34:LEU:HD22 | 1.88 | 0.56 |
| 8:RI:92:VAL:HG13 | 8:RI:120:ILE:HB | 1.86 | 0.56 |
| 32:XA:719:C:O2' | 49:XR:49:LYS:HB3 | 2.05 | 0.56 |
| 5:YF:164:ARG:HD2 | 5:YF:175:THR:HG23 | 1.88 | 0.56 |
| 32:QA:187:C:O2' | 51:QT:89:ARG:NH2 | 2.34 | 0.56 |
| 32:QA:343:U:O2' | 32:QA:346:G:O6 | 2.15 | 0.56 |
| 32:QA:1239:A:O2' | 38:QG:114:ARG:O | 2.21 | 0.56 |
| 40:QI:108:VAL:HG12 | 40:QI:109:VAL:H | 1.71 | 0.56 |
| 1:RA:1076:C:H1' | 1:RA:1077:A:H5' | 1.86 | 0.56 |
| 1:RA:1798:U:H5' | 3:RD:259:THR:CG2 | 2.36 | 0.56 |
| 20:RY:92:ASN:N | 20:RY:93:GLY:HA2 | 2.21 | 0.56 |
| 32:XA:1053:G:N7 | 32:XA:1200:C:H5'' | 2.21 | 0.56 |
| 1:YA:1062:G:O2' | 1:YA:1063:G:H5' | 2.06 | 0.56 |
| 1:YA:1124:C:H2' | 1:YA:1125:G:O4' | 2.06 | 0.56 |
| 1:YA:1028:A:H62 | 1:YA:1126:A:H8 | 1.53 | 0.56 |
| 21:YZ:91:LEU:HG | 21:YZ:130:PRO:HG3 | 1.87 | 0.56 |
| 48:QQ:78:GLU:HG2 | 48:QQ:79:SER:H | 1.71 | 0.56 |
| 1:RA:2464:C:H2' | 1:RA:2465:C:O4' | 2.05 | 0.56 |
| 21:RZ:72:ARG:CG | 21:RZ:89:PHE:HB2 | 2.35 | 0.56 |
| 1:YA:323:G:H1' | 1:YA:1205:U:O2 | 2.06 | 0.56 |
| 1:RA:2094:G:P | 8:RI:22:LYS:HD2 | 2.46 | 0.55 |
| 1:RA:2171:A:H4' | 1:RA:2172:U:OP1 | 2.06 | 0.55 |
| 1:YA:1889:A:N1 | 1:YA:2234:G:H1' | 2.21 | 0.55 |
| 32:QA:110:C:O2' | 47:QP:25:ARG:O | 2.22 | 0.55 |
| 53:QV:4:G:HO2' | 53:QV:5:G:H8 | 1.53 | 0.55 |
| 1:RA:2321:G:O2' | 1:RA:2322:A:OP1 | 2.23 | 0.55 |
| 4:RE:51:PHE:H | 4:RE:75:VAL:CG1 | 2.19 | 0.55 |
| 32:XA:142:G:H2' | 32:XA:143:A:H8 | 1.72 | 0.55 |
| 32:XA:411:A:OP2 | 35:XD:25:ARG:NH2 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:XA:444:C:H42 | 32:XA:490:G:H1 | 1.54 | 0.55 |
| 49:XR:56:THR:HB | 49:XR:58:LEU:HD23 | 1.87 | 0.55 |
| 1:YA:1364:G:P | 23:Y1:3:LYS:HG3 | 2.46 | 0.55 |
| 1:YA:2659:G:O2' | 7:YH:175:LYS:HE2 | 2.06 | 0.55 |
| 1:RA:212:G:H2' | 1:RA:213:A:O4' | 2.07 | 0.55 |
| 49:XR:59:SER:OG | 49:XR:62:GLU:HG2 | 2.06 | 0.55 |
| 1:YA:300:A:H2' | 1:YA:334:C:H1' | 1.87 | 0.55 |
| 16:YU:108:GLU:O | 16:YU:112:ARG:HG2 | 2.06 | 0.55 |
| 19:RX:53:LYS:HB3 | 19:RX:82:GLN:HB3 | 1.87 | 0.55 |
| 32:XA:1030(A):C:N3 | 32:XA:1031:G:N2 | 2.54 | 0.55 |
| 32:XA:1047:G:OP1 | 45:YN:4:LYS:NZ | 2.34 | 0.55 |
| 55:XY:108:GLU:HA | 55:XY:170:GLY:HA2 | 1.89 | 0.55 |
| 1:YA:528:A:OP2 | 9:YN:114:ARG:NH1 | 2.39 | 0.55 |
| 33:QB:21:ARG:H | 33:QB:21:ARG:CD | 2.20 | 0.55 |
| 1:RA:2810:A:N6 | 1:RA:2891:G:O2' | 2.34 | 0.55 |
| 1:RA:1800:C:OP2 | 3:RD:183:ARG:NH2 | 2.40 | 0.55 |
| 4:RE:170:LEU:HB3 | 4:RE:184:VAL:HG22 | 1.89 | 0.55 |
| 26:Y4:61:ARG:HH22 | 50:XS:9:VAL:HG21 | 1.71 | 0.55 |
| 5:YF:132:VAL:HG21 | 5:YF:163:VAL:HG22 | 1.89 | 0.55 |
| 7:YH:89:ILE:O | 7:YH:129:THR:HG23 | 2.06 | 0.55 |
| 35:QD:13:ARG:NH1 | 35:QD:38:TYR:O | 2.40 | 0.55 |
| 1:RA:1050:A:C2 | 1:RA:2751:G:C2 | 2.95 | 0.55 |
| 1:RA:588:U:H2' | 1:RA:589:C:C6 | 2.41 | 0.55 |
| 6:RG:50:ALA:C | 6:RG:52:ILE:H | 2.10 | 0.55 |
| 12:YQ:45:GLN:N | 12:YQ:45:GLN:OE1 | 2.37 | 0.55 |
| 32:QA:1187:G:H4' | 40:QI:111:ARG:HH11 | 1.71 | 0.55 |
| 46:QO:74:ASP:OD2 | 46:QO:77:ARG:HG3 | 2.07 | 0.55 |
| 1:RA:250:G:P | 30:R8:13:ARG:HH22 | 2.30 | 0.55 |
| 1:RA:1049:C:H2' | 1:RA:1050:A:C8 | 2.42 | 0.55 |
| 1:RA:1688:U:O2 | 1:RA:1700:A:H5' | 2.06 | 0.55 |
| 40:XI:53:VAL:C | 40:XI:55:ALA:H | 2.07 | 0.55 |
| 46:XO:74:ASP:OD2 | 46:XO:77:ARG:HG3 | 2.06 | 0.55 |
| 3:YD:69:ARG:NH2 | 3:YD:128:GLY:O | 2.32 | 0.55 |
| 8:YI:130:TYR:HB3 | 8:YI:138:ILE:HB | 1.88 | 0.55 |
| 19:YX:53:LYS:HB3 | 19:YX:82:GLN:HB3 | 1.88 | 0.55 |
| 8:RI:38:LEU:HD12 | 8:RI:38:LEU:H | 1.72 | 0.55 |
| 11:RP:98:GLU:OE1 | 11:RP:102:ARG:NH1 | 2.30 | 0.55 |
| 53:XV:9:G:O2' | 53:XV:10:G:N7 | 2.37 | 0.55 |
| 1:YA:2128:C:H5' | 1:YA:2129:C:OP2 | 2.07 | 0.55 |
| 6:YG:11:TYR:HA | 6:YG:15:VAL:HB | 1.88 | 0.55 |
| 21:YZ:125:LEU:HB3 | 21:YZ:165:VAL:HG13 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:QB:158:LEU:HG | 33:QB:182:ILE:HD11 | 1.89 | 0.55 |
| 44:QM:3:ARG:HD2 | 44:QM:9:ILE:HG12 | 1.88 | 0.55 |
| 23:R1:64:ALA:HA | 23:R1:67:ILE:HG13 | 1.89 | 0.55 |
| 1:RA:2142:C:H2' | 1:RA:2143:C:C6 | 2.42 | 0.55 |
| 1:RA:84:A:H5'' | 20:RY:8:LYS:HE2 | 1.88 | 0.55 |
| 21:RZ:126:VAL:CG1 | 21:RZ:161:VAL:HG23 | 2.37 | 0.55 |
| 35:XD:150:GLU:HA | 35:XD:153:ARG:HE | 1.72 | 0.55 |
| 1:YA:1087:G:H1 | 1:YA:1102:C:N4 | 2.04 | 0.55 |
| 1:YA:607:U:OP1 | 5:YF:102:PRO:HA | 2.07 | 0.55 |
| 32:XA:438:G:O2' | 32:XA:494:U:O4 | 2.23 | 0.55 |
| 35:XD:13:ARG:NH1 | 35:XD:38:TYR:O | 2.40 | 0.55 |
| 9:RN:94:HIS:HB3 | 9:RN:97:ARG:HD3 | 1.89 | 0.54 |
| 13:RR:67:LEU:HD13 | 13:RR:76:VAL:HG21 | 1.89 | 0.54 |
| 33:XB:84:GLU:HB3 | 33:XB:219:VAL:HG21 | 1.89 | 0.54 |
| 32:XA:922:G:H4' | 36:XE:20:GLN:HA | 1.89 | 0.54 |
| 39:XH:64:LYS:HG2 | 39:XH:79:VAL:HG21 | 1.88 | 0.54 |
| 34:XC:12:LEU:HD11 | 45:XN:51:GLY:HA2 | 1.89 | 0.54 |
| 23:Y1:64:ALA:HA | 23:Y1:67:ILE:HG13 | 1.89 | 0.54 |
| 1:YA:82:G:N1 | 1:YA:103:A:OP2 | 2.35 | 0.54 |
| 1:YA:1075:C:H2' | 1:YA:1076:C:H5' | 1.90 | 0.54 |
| 1:YA:2189:U:H2' | 1:YA:2190:G:C8 | 2.42 | 0.54 |
| 1:YA:276:A:H5'' | 1:YA:277:C:H5' | 1.89 | 0.54 |
| 1:YA:747:U:O2 | 1:YA:2014:A:H1' | 2.08 | 0.54 |
| 32:QA:1391:U:H2' | 32:QA:1392:G:C8 | 2.42 | 0.54 |
| 46:QO:84:LYS:O | 46:QO:84:LYS:HD3 | 2.06 | 0.54 |
| 1:RA:1721:G:H2' | 1:RA:1740:G:O6 | 2.07 | 0.54 |
| 1:RA:764:A:H5' | 3:RD:210:GLY:HA2 | 1.88 | 0.54 |
| 5:RF:140:LEU:HD21 | 5:RF:170:LEU:HD11 | 1.88 | 0.54 |
| 9:RN:4:TYR:CD2 | 16:RU:100:VAL:HG11 | 2.42 | 0.54 |
| 20:RY:87:LYS:HB3 | 20:RY:95:LYS:HD3 | 1.90 | 0.54 |
| 33:XB:44:LEU:H | 33:XB:44:LEU:HD22 | 1.73 | 0.54 |
| 1:YA:2127:G:H2' | 1:YA:2128:C:O4' | 2.07 | 0.54 |
| 1:YA:2142:C:H2' | 1:YA:2143:C:C6 | 2.41 | 0.54 |
| 39:QH:10:LEU:HD22 | 39:QH:83:ILE:HD11 | 1.89 | 0.54 |
| 50:QS:22:LEU:HD22 | 50:QS:28:LYS:HA | 1.89 | 0.54 |
| 1:RA:1086:A:OP1 | 1:RA:1104:C:O2' | 2.24 | 0.54 |
| 1:RA:2110:G:H5'' | 1:RA:2111:C:H5 | 1.73 | 0.54 |
| 1:RA:2128:C:H5' | 1:RA:2129:C:OP2 | 2.07 | 0.54 |
| 32:XA:406:G:H5' | 35:XD:5:ILE:HD11 | 1.88 | 0.54 |
| 32:XA:503:C:OP2 | 43:XL:116:SER:HB3 | 2.07 | 0.54 |
| 32:XA:632:A:H5' | 32:XA:633:G:OP2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 39:XH:12:ARG:HD2 | 39:XH:26:VAL:HG12 | 1.89 | 0.54 |
| 1:YA:1359:A:H61 | 1:YA:1372:U:H3 | 1.54 | 0.54 |
| 15:YT:65:LYS:HE3 | 15:YT:67:SER:HB2 | 1.90 | 0.54 |
| 32:QA:324:G:N1 | 32:QA:327:A:OP2 | 2.40 | 0.54 |
| 32:QA:38:G:N2 | 32:QA:397:A:H5' | 2.21 | 0.54 |
| 32:QA:396:G:O2' | 32:QA:398:C:OP1 | 2.15 | 0.54 |
| 32:QA:261:U:OP2 | 51:QT:79:ARG:NH2 | 2.40 | 0.54 |
| 1:RA:2189:U:H2' | 1:RA:2190:G:C8 | 2.42 | 0.54 |
| 1:RA:2445:G:OP1 | 5:RF:74:ARG:NH2 | 2.38 | 0.54 |
| 1:RA:1803:A:O2' | 3:RD:259:THR:HG21 | 2.07 | 0.54 |
| 1:YA:1032:A:H4' | 31:Y9:16:VAL:HG11 | 1.88 | 0.54 |
| 1:YA:2099:U:H3 | 1:YA:2190:G:H1 | 1.54 | 0.54 |
| 1:YA:2327:A:H2' | 1:YA:2328:A:C8 | 2.42 | 0.54 |
| 1:YA:265:A:N1 | 1:YA:427:U:O2' | 2.33 | 0.54 |
| 3:YD:30:GLU:HG3 | 3:YD:94:LEU:HD21 | 1.90 | 0.54 |
| 15:YT:95:ARG:HG2 | 15:YT:95:ARG:HH11 | 1.73 | 0.54 |
| 32:QA:921:U:O2' | 36:QE:19:MET:O | 2.12 | 0.54 |
| 19:RX:5:TYR:O | 24:R2:36:ARG:NH2 | 2.39 | 0.54 |
| 1:RA:747:U:O2 | 1:RA:2014:A:H1' | 2.08 | 0.54 |
| 32:XA:1510:U:H2' | 32:XA:1511:G:C8 | 2.43 | 0.54 |
| 1:YA:1184:G:OP1 | 25:Y3:30:ARG:HD2 | 2.07 | 0.54 |
| 6:YG:113:ARG:HH21 | 26:Y4:33:VAL:HG12 | 1.71 | 0.54 |
| 1:YA:1341:U:OP1 | 1:YA:1397:U:N3 | 2.33 | 0.54 |
| 3:YD:10:THR:OG1 | 3:YD:13:ARG:HG2 | 2.08 | 0.54 |
| 1:YA:601:C:OP1 | 5:YF:108:LYS:HE3 | 2.07 | 0.54 |
| 13:RR:36:THR:HG22 | 13:RR:37:THR:H | 1.73 | 0.54 |
| 32:XA:1157:A:H5' | 32:XA:1158:C:C6 | 2.43 | 0.54 |
| 41:XJ:37:PRO:HA | 41:XJ:72:VAL:HG12 | 1.89 | 0.54 |
| 41:XJ:57:LYS:HE2 | 41:XJ:60:ARG:NH2 | 2.23 | 0.54 |
| 1:YA:1250:G:N7 | 11:YP:18:ARG:NH2 | 2.55 | 0.54 |
| 32:QA:1003:G:N2 | 32:QA:1004:A:H1' | 2.23 | 0.54 |
| 32:QA:1442(A):G:N3 | 32:QA:1442(A):G:H2' | 2.23 | 0.54 |
| 32:QA:1055:A:O2' | 34:QC:161:GLU:O | 2.18 | 0.54 |
| 35:QD:81:GLU:O | 35:QD:85:LYS:HB2 | 2.08 | 0.54 |
| 32:QA:1279:A:H5'' | 41:QJ:7:LYS:NZ | 2.23 | 0.54 |
| 37:QF:97:PHE:HB2 | 49:QR:32:ARG:HD2 | 1.90 | 0.54 |
| 25:R3:8:LEU:HD12 | 25:R3:31:LEU:HA | 1.89 | 0.54 |
| 26:R4:41:PRO:HG3 | 26:R4:49:PHE:CE1 | 2.42 | 0.54 |
| 1:RA:1036:G:H1 | 1:RA:1119:C:H42 | 1.55 | 0.54 |
| 1:RA:2336:A:H61 | 22:R0:43:THR:HG22 | 1.73 | 0.54 |
| 32:XA:1030(B):G:H2' | 32:XA:1030(C):C:H5'' | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:XA:1131:G:H2' | 32:XA:1132:C:C6 | 2.43 | 0.54 |
| 1:YA:1049:C:O2 | 1:YA:1113:U:H4' | 2.07 | 0.54 |
| 1:YA:1101:U:H2' | 1:YA:1102:C:C6 | 2.43 | 0.54 |
| 1:YA:2461:C:H2' | 1:YA:2462:U:C6 | 2.43 | 0.54 |
| 17:YV:43:GLU:N | 17:YV:43:GLU:OE2 | 2.41 | 0.54 |
| 40:QI:49:PRO:HD2 | 40:QI:81:ILE:HD11 | 1.89 | 0.54 |
| 1:RA:2354:G:H21 | 22:R0:36:ILE:HD11 | 1.73 | 0.54 |
| 25:R3:3:ARG:NH1 | 25:R3:60:GLU:OE2 | 2.36 | 0.54 |
| 1:RA:2152:G:H2' | 1:RA:2153:G:C8 | 2.42 | 0.54 |
| 1:RA:2507:C:O4' | 55:QY:238:ASN:HB3 | 2.08 | 0.54 |
| 3:RD:108:PRO:HD2 | 3:RD:111:LEU:HG | 1.88 | 0.54 |
| 4:RE:73:GLU:CD | 4:RE:73:GLU:H | 2.10 | 0.54 |
| 9:RN:128:HIS:O | 9:RN:131:GLN:NE2 | 2.40 | 0.54 |
| 32:XA:1239:A:H62 | 32:XA:1299:A:H62 | 1.56 | 0.54 |
| 32:XA:692:U:O2' | 32:XA:694:A:N7 | 2.27 | 0.54 |
| 35:XD:173:TRP:CD1 | 35:XD:189:PRO:HG3 | 2.42 | 0.54 |
| 45:XN:4:LYS:HG3 | 45:XN:7:ILE:HD11 | 1.90 | 0.54 |
| 51:XT:60:GLU:HG3 | 51:XT:81:LYS:HD2 | 1.89 | 0.54 |
| 1:YA:2262:U:H4' | 1:YA:2328:A:C2 | 2.42 | 0.54 |
| 5:YF:167:ALA:HB1 | 5:YF:173:VAL:HG11 | 1.88 | 0.54 |
| 5:YF:184:TYR:O | 5:YF:188:ARG:HG3 | 2.07 | 0.54 |
| 40:QI:16:ARG:HD3 | 40:QI:64:THR:HG21 | 1.89 | 0.54 |
| 55:QY:106:ASP:HA | 55:QY:109:ARG:HD3 | 1.90 | 0.54 |
| 4:RE:78:LEU:O | 4:RE:79:ARG:NH1 | 2.36 | 0.54 |
| 6:RG:116:ASP:OD1 | 44:QM:68:GLY:HA3 | 2.07 | 0.54 |
| 9:RN:46:VAL:HG23 | 9:RN:48:MET:HG2 | 1.90 | 0.54 |
| 32:XA:1151:A:O2' | 32:XA:1152:A:H8 | 1.90 | 0.54 |
| 34:XC:150:LYS:HG3 | 34:XC:169:ALA:HB2 | 1.90 | 0.54 |
| 32:XA:1106:G:H5' | 34:XC:172:ARG:HG2 | 1.89 | 0.54 |
| 38:XG:132:GLY:O | 38:XG:136:LYS:HG2 | 2.06 | 0.54 |
| 32:XA:452:A:N3 | 47:XP:72:ARG:NH1 | 2.56 | 0.54 |
| 1:YA:517:C:OP1 | 27:Y5:16:ARG:NH2 | 2.41 | 0.54 |
| 30:Y8:63:PRO:HG2 | 30:Y8:64:TYR:CE2 | 2.42 | 0.54 |
| 6:YG:18:GLU:OE1 | 6:YG:21:ARG:NH2 | 2.40 | 0.54 |
| 51:QT:47:GLY:HA2 | 51:QT:48:LYS:HB2 | 1.88 | 0.54 |
| 1:RA:2115:G:H21 | 1:RA:2171:A:H61 | 1.55 | 0.54 |
| 32:XA:1015:A:H2' | 32:XA:1016:A:C8 | 2.43 | 0.54 |
| 32:XA:979:C:H42 | 45:XN:18:VAL:HG12 | 1.73 | 0.54 |
| 33:XB:54:THR:HG21 | 33:XB:201:ILE:HD11 | 1.89 | 0.54 |
| 44:XM:95:GLY:O | 44:XM:110:ARG:HG3 | 2.08 | 0.54 |
| 1:YA:774:A:N3 | 1:YA:774:A:H2' | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:YG:11:TYR:OH | 6:YG:33:ARG:HG3 | 2.08 | 0.54 |
| 55:QY:245:ARG:HB2 | 55:QY:256:GLU:HB3 | 1.90 | 0.53 |
| 5:RF:178:PRO:HB2 | 5:RF:201:VAL:CG2 | 2.38 | 0.53 |
| 8:RI:130:TYR:HB3 | 8:RI:138:ILE:HB | 1.89 | 0.53 |
| 35:XD:173:TRP:CD1 | 35:XD:174:LEU:HG | 2.43 | 0.53 |
| 55:XY:119:THR:H | 55:XY:302:ASP:CG | 2.11 | 0.53 |
| 55:XY:177:PHE:HB3 | 55:XY:321:ARG:HH22 | 1.74 | 0.53 |
| 32:QA:411:A:OP2 | 35:QD:25:ARG:NH2 | 2.41 | 0.53 |
| 33:QB:15:VAL:HG23 | 33:QB:209:ARG:HB3 | 1.89 | 0.53 |
| 42:QK:99:GLN:HG2 | 42:QK:105:VAL:HG21 | 1.90 | 0.53 |
| 1:RA:1029:A:OP1 | 12:RQ:128:LYS:NZ | 2.40 | 0.53 |
| 1:RA:2502:G:H5'' | 1:RA:2503:2MA:H5'' | 1.89 | 0.53 |
| 5:RF:53:THR:HG22 | 5:RF:55:GLY:H | 1.74 | 0.53 |
| 13:RR:24:GLN:HB3 | 13:RR:44:LEU:HD11 | 1.90 | 0.53 |
| 32:XA:324:G:N1 | 32:XA:327:A:OP2 | 2.40 | 0.53 |
| 36:XE:57:LYS:HG2 | 36:XE:61:TYR:HE2 | 1.72 | 0.53 |
| 41:XJ:5:ARG:N | 41:XJ:99:LYS:O | 2.40 | 0.53 |
| 32:XA:1492:A:OP2 | 43:XL:47:LYS:HG3 | 2.09 | 0.53 |
| 30:Y8:6:THR:HG23 | 30:Y8:64:TYR:HD2 | 1.73 | 0.53 |
| 1:YA:2022:U:O2' | 1:YA:2617:C:H5' | 2.08 | 0.53 |
| 1:YA:998:C:OP2 | 16:YU:92:ARG:NH2 | 2.41 | 0.53 |
| 19:YX:65:ARG:HB3 | 19:YX:70:LEU:HD23 | 1.89 | 0.53 |
| 33:QB:76:GLN:NE2 | 33:QB:206:ASP:OD1 | 2.42 | 0.53 |
| 35:QD:15:GLU:HG3 | 35:QD:63:LYS:HD3 | 1.91 | 0.53 |
| 36:QE:110:LEU:HD13 | 36:QE:118:ILE:HG21 | 1.89 | 0.53 |
| 39:QH:86:ILE:HG13 | 39:QH:133:LEU:HD22 | 1.90 | 0.53 |
| 1:RA:185:U:H4' | 1:RA:218:A:H4' | 1.91 | 0.53 |
| 32:XA:404:U:C5' | 35:XD:122:ARG:HD3 | 2.38 | 0.53 |
| 1:YA:299:A:N1 | 1:YA:322:A:O2' | 2.37 | 0.53 |
| 32:QA:1068:G:H8 | 32:QA:1068:G:OP2 | 1.91 | 0.53 |
| 32:QA:355:C:O2' | 32:QA:388:G:N3 | 2.29 | 0.53 |
| 46:QO:17:ARG:HD3 | 46:QO:26:GLU:OE1 | 2.09 | 0.53 |
| 1:RA:2022:U:O2' | 1:RA:2617:C:H5' | 2.08 | 0.53 |
| 32:XA:1402:4OC:HM22 | 32:XA:1403:C:H5' | 1.90 | 0.53 |
| 32:XA:975:A:N1 | 41:XJ:48:THR:HB | 2.24 | 0.53 |
| 40:XI:4:TYR:HB2 | 40:XI:19:LEU:HB2 | 1.91 | 0.53 |
| 40:XI:22:GLY:HA3 | 40:XI:60:ASP:OD1 | 2.07 | 0.53 |
| 32:XA:707:C:OP1 | 42:XK:85:ARG:NH1 | 2.41 | 0.53 |
| 52:XU:5:ASP:O | 52:XU:11:GLY:HA3 | 2.09 | 0.53 |
| 1:YA:2313:C:H2' | 1:YA:2314:C:C6 | 2.43 | 0.53 |
| 8:YI:114:LEU:HD12 | 8:YI:116:LEU:HB2 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:YT:39:ARG:HH22 | 32:XA:344:A:H4' | 1.73 | 0.53 |
| 32:QA:1030(A):C:N3 | 32:QA:1031:G:N2 | 2.56 | 0.53 |
| 1:RA:1031:G:O2' | 31:R9:7:VAL:O | 2.24 | 0.53 |
| 6:RG:77:ILE:HG21 | 6:RG:80:PHE:CD2 | 2.43 | 0.53 |
| 32:XA:17:U:O2' | 32:XA:1079:G:H1' | 2.07 | 0.53 |
| 33:XB:69:LEU:HB3 | 33:XB:162:ILE:HG22 | 1.90 | 0.53 |
| 32:XA:942:G:H21 | 40:XI:124:GLN:NE2 | 2.05 | 0.53 |
| 1:YA:1048:A:N1 | 1:YA:1112:G:O2' | 2.30 | 0.53 |
| 1:YA:1471:A:OP2 | 1:YA:1519:G:N2 | 2.38 | 0.53 |
| 1:YA:2478:A:OP2 | 31:Y9:2:LYS:NZ | 2.22 | 0.53 |
| 1:RA:1075:C:H2' | 1:RA:1076:C:H5' | 1.89 | 0.53 |
| 1:RA:1087:G:N2 | 1:RA:1102:C:N3 | 2.44 | 0.53 |
| 1:RA:1824:G:O3' | 3:RD:249:PRO:HD3 | 2.09 | 0.53 |
| 1:RA:2526:G:H5' | 1:RA:2742:C:O2' | 2.09 | 0.53 |
| 32:XA:1006:C:H2' | 32:XA:1007:C:C6 | 2.43 | 0.53 |
| 41:XJ:61:GLU:OE1 | 45:XN:58:LYS:NZ | 2.38 | 0.53 |
| 55:XY:184:VAL:HG23 | 55:XY:200:ALA:HA | 1.90 | 0.53 |
| 1:YA:1991:U:H2' | 1:YA:1992:G:H5'' | 1.91 | 0.53 |
| 32:QA:1158:C:H5 | 32:QA:1181:G:H1 | 1.55 | 0.53 |
| 44:QM:34:LEU:HD13 | 44:QM:41:PRO:HA | 1.89 | 0.53 |
| 1:RA:2756:U:H5'' | 31:R9:19:ARG:HA | 1.91 | 0.53 |
| 1:RA:1171:G:N2 | 1:RA:1178:C:O2 | 2.42 | 0.53 |
| 1:RA:1889:A:H2' | 1:RA:1890:A:C8 | 2.44 | 0.53 |
| 1:RA:2311:A:C6 | 6:RG:80:PHE:HB3 | 2.44 | 0.53 |
| 32:XA:1029:C:N4 | 32:XA:1030(A):C:H41 | 2.07 | 0.53 |
| 1:YA:1101:U:H2' | 1:YA:1102:C:H6 | 1.73 | 0.53 |
| 15:YT:108:ARG:NH1 | 32:XA:1464:G:OP1 | 2.41 | 0.53 |
| 53:QV:19:G:H5' | 53:QV:20:U:C5 | 2.44 | 0.53 |
| 55:QY:328:ARG:HH22 | 55:QY:340:LEU:N | 2.06 | 0.53 |
| 1:RA:1062:G:N7 | 1:RA:1070:A:H1' | 2.24 | 0.53 |
| 32:XA:1157:A:H4' | 32:XA:1158:C:O5' | 2.09 | 0.53 |
| 38:XG:113:GLU:HG3 | 38:XG:118:VAL:HG12 | 1.91 | 0.53 |
| 1:YA:2171:A:H4' | 1:YA:2172:U:OP1 | 2.07 | 0.53 |
| 1:YA:2805:G:H2' | 1:YA:2807:G:C8 | 2.43 | 0.53 |
| 13:YR:36:THR:HG22 | 13:YR:37:THR:H | 1.73 | 0.53 |
| 32:QA:1412:C:H2' | 32:QA:1413:A:C8 | 2.44 | 0.53 |
| 32:XA:737:A:H2' | 32:XA:738:C:C6 | 2.44 | 0.53 |
| 33:XB:71:VAL:HG12 | 33:XB:93:VAL:HG22 | 1.91 | 0.53 |
| 40:XI:26:VAL:HA | 40:XI:61:ALA:O | 2.09 | 0.53 |
| 1:YA:2345:G:H1' | 1:YA:2382:G:H5' | 1.90 | 0.53 |
| 4:YE:111:ARG:HG3 | 4:YE:160:TYR:CD2 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:YF:184:TYR:CE2 | 5:YF:188:ARG:HD2 | 2.43 | 0.53 |
| 32:QA:1033:G:H2' | 32:QA:1034:G:H8 | 1.74 | 0.53 |
| 39:QH:86:ILE:HG21 | 39:QH:133:LEU:HD13 | 1.91 | 0.53 |
| 22:R0:27:GLU:HG3 | 22:R0:68:GLU:HA | 1.91 | 0.53 |
| 32:XA:1347:G:N2 | 32:XA:1373:G:H2' | 2.24 | 0.53 |
| 24:Y2:16:LEU:O | 24:Y2:67:LYS:NZ | 2.41 | 0.53 |
| 1:YA:1062:G:N7 | 1:YA:1070:A:H1' | 2.24 | 0.53 |
| 12:YQ:7:MET:HG3 | 12:YQ:9:TYR:O | 2.09 | 0.53 |
| 17:YV:29:PRO:HA | 17:YV:61:VAL:HG23 | 1.91 | 0.53 |
| 40:QI:33:PHE:HE1 | 40:QI:43:ALA:HB1 | 1.74 | 0.52 |
| 1:RA:273(A):G:H4' | 1:RA:273(B):U:H5'' | 1.90 | 0.52 |
| 1:RA:300:A:H2' | 1:RA:334:C:H1' | 1.90 | 0.52 |
| 44:XM:54:VAL:HA | 44:XM:57:ARG:HB3 | 1.91 | 0.52 |
| 26:Y4:53:GLU:CD | 26:Y4:53:GLU:H | 2.13 | 0.52 |
| 1:YA:1378:A:OP1 | 29:Y7:10:ARG:NH2 | 2.42 | 0.52 |
| 1:YA:1406:U:H2' | 1:YA:1407:C:C6 | 2.44 | 0.52 |
| 1:YA:2893:G:H5'' | 1:YA:2894:G:O4' | 2.09 | 0.52 |
| 1:YA:321:G:OP2 | 5:YF:135:LYS:HD3 | 2.09 | 0.52 |
| 11:YP:100:LEU:HD12 | 11:YP:112:LEU:HD11 | 1.90 | 0.52 |
| 20:YY:82:PRO:O | 20:YY:101:LYS:NZ | 2.27 | 0.52 |
| 44:QM:3:ARG:HG3 | 44:QM:4:ILE:N | 2.23 | 0.52 |
| 1:RA:2836:U:H2' | 1:RA:2837:G:C8 | 2.44 | 0.52 |
| 1:RA:922:U:H2' | 1:RA:923:C:C6 | 2.44 | 0.52 |
| 19:RX:11:PRO:HB3 | 19:RX:92:LEU:HD11 | 1.91 | 0.52 |
| 36:XE:12:LEU:HB3 | 36:XE:31:LEU:HB2 | 1.91 | 0.52 |
| 41:XJ:9:ARG:NH2 | 41:XJ:95:GLU:OE1 | 2.42 | 0.52 |
| 1:YA:2659:G:H4' | 7:YH:175:LYS:HD3 | 1.91 | 0.52 |
| 17:YV:52:VAL:HG23 | 17:YV:55:ALA:HB3 | 1.90 | 0.52 |
| 32:QA:376:G:H5'' | 47:QP:5:ARG:HD3 | 1.91 | 0.52 |
| 49:QR:33:ASP:OD2 | 49:QR:36:ASN:HB2 | 2.10 | 0.52 |
| 34:XC:164:ARG:NH1 | 34:XC:166:GLU:OE1 | 2.42 | 0.52 |
| 32:XA:1129:C:OP1 | 40:XI:16:ARG:NH1 | 2.43 | 0.52 |
| 1:YA:1110:G:H1' | 1:YA:1111:A:C8 | 2.44 | 0.52 |
| 1:YA:2206:G:H5'' | 1:YA:2207:G:N7 | 2.24 | 0.52 |
| 5:YF:103:LYS:O | 5:YF:106:ARG:HG2 | 2.10 | 0.52 |
| 7:YH:143:GLN:NE2 | 7:YH:147:ASN:OD1 | 2.42 | 0.52 |
| 17:YV:72:VAL:HG13 | 17:YV:85:LYS:HB3 | 1.90 | 0.52 |
| 32:QA:176:C:H2' | 32:QA:177:C:C6 | 2.44 | 0.52 |
| 26:R4:59:PHE:HE1 | 50:QS:64:GLU:HA | 1.75 | 0.52 |
| 51:QT:10:LEU:HB3 | 51:QT:12:ALA:H | 1.74 | 0.52 |
| 1:RA:1084:A:H3' | 1:RA:1085:A:C4' | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:RX:2:LYS:NZ | 19:RX:38:GLU:OE2 | 2.23 | 0.52 |
| 32:XA:977:A:N6 | 32:XA:1224:G:OP1 | 2.38 | 0.52 |
| 33:XB:16:HIS:HB2 | 33:XB:204:ASN:HB3 | 1.90 | 0.52 |
| 40:XI:24:GLY:HA2 | 40:XI:59:PHE:O | 2.10 | 0.52 |
| 55:XY:174:ARG:NH1 | 55:XY:338:ASP:OD1 | 2.43 | 0.52 |
| 1:YA:1300:U:H4' | 1:YA:1301:A:H5' | 1.92 | 0.52 |
| 1:YA:2104:G:N2 | 1:YA:2105:C:C4 | 2.77 | 0.52 |
| 1:YA:922:U:H2' | 1:YA:923:C:C6 | 2.44 | 0.52 |
| 10:YO:80:ASP:OD1 | 15:YT:64:ARG:NH2 | 2.40 | 0.52 |
| 32:QA:410:G:OP1 | 35:QD:30:LYS:NZ | 2.32 | 0.52 |
| 34:QC:148:GLY:HA3 | 34:QC:172:ARG:O | 2.09 | 0.52 |
| 1:RA:2206:G:H8 | 1:RA:2207:G:N7 | 2.08 | 0.52 |
| 1:RA:272(E):U:H2' | 1:RA:272(F):C:C6 | 2.44 | 0.52 |
| 1:RA:514:A:N3 | 1:RA:581:C:O2' | 2.40 | 0.52 |
| 32:XA:457:C:H2' | 32:XA:458:C:H6 | 1.75 | 0.52 |
| 35:XD:15:GLU:HG3 | 35:XD:63:LYS:HD3 | 1.91 | 0.52 |
| 1:YA:1067:A:H4' | 1:YA:1068:G:OP2 | 2.09 | 0.52 |
| 6:YG:36:LYS:HE2 | 6:YG:95:ARG:NH1 | 2.24 | 0.52 |
| 1:YA:2752:C:OP2 | 7:YH:4:ILE:HD11 | 2.09 | 0.52 |
| 9:YN:62:VAL:CG1 | 9:YN:66:LYS:HB2 | 2.40 | 0.52 |
| 13:YR:67:LEU:HD13 | 13:YR:76:VAL:HG21 | 1.92 | 0.52 |
| 21:YZ:72:ARG:CG | 21:YZ:89:PHE:HB2 | 2.39 | 0.52 |
| 32:QA:328:C:H4' | 32:QA:329:A:H5' | 1.92 | 0.52 |
| 33:QB:82:ARG:HG3 | 33:QB:92:TYR:CZ | 2.43 | 0.52 |
| 34:QC:22:TRP:CZ2 | 45:QN:54:PRO:HG2 | 2.44 | 0.52 |
| 11:RP:63:PRO:HD3 | 30:R8:27:THR:HG22 | 1.91 | 0.52 |
| 1:RA:1038:C:N4 | 1:RA:1117:G:H1 | 2.06 | 0.52 |
| 1:RA:1165:U:H2' | 1:RA:1166:C:C6 | 2.45 | 0.52 |
| 14:RS:14:VAL:O | 14:RS:18:ILE:HG12 | 2.10 | 0.52 |
| 14:RS:15:ARG:O | 14:RS:19:LYS:HG2 | 2.08 | 0.52 |
| 32:XA:1002:G:N3 | 32:XA:1003:G:H8 | 2.07 | 0.52 |
| 32:XA:841:U:OP1 | 32:XA:841:U:H6 | 1.92 | 0.52 |
| 40:XI:8:GLY:HA3 | 40:XI:76:ALA:O | 2.09 | 0.52 |
| 44:XM:6:GLY:HA3 | 44:XM:67:GLU:HG3 | 1.92 | 0.52 |
| 46:XO:17:ARG:HD3 | 46:XO:26:GLU:OE1 | 2.10 | 0.52 |
| 49:XR:32:ARG:HA | 49:XR:69:THR:HG21 | 1.92 | 0.52 |
| 1:YA:154(B):C:H42 | 1:YA:171:G:H1 | 1.57 | 0.52 |
| 1:YA:212:G:H2' | 1:YA:213:A:O4' | 2.10 | 0.52 |
| 2:YB:14:U:OP2 | 2:YB:70:C:O2' | 2.21 | 0.52 |
| 32:QA:457:C:H2' | 32:QA:458:C:H6 | 1.74 | 0.52 |
| 41:QJ:8:LEU:HB2 | 41:QJ:70:ARG:HB2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:QO:25:THR:HG21 | 46:QO:70:LEU:HB2 | 1.91 | 0.52 |
| 1:RA:2023:G:H5' | 1:RA:2617:C:H4' | 1.91 | 0.52 |
| 1:RA:586:A:N1 | 1:RA:809:G:O2' | 2.38 | 0.52 |
| 18:RW:23:LEU:HD11 | 27:R5:25:LEU:HB2 | 1.92 | 0.52 |
| 32:XA:1456:G:O3' | 51:XT:39:LYS:NZ | 2.43 | 0.52 |
| 1:YA:2756:U:OP2 | 31:Y9:19:ARG:NE | 2.30 | 0.52 |
| 1:YA:637:A:OP1 | 11:YP:133:SER:OG | 2.24 | 0.52 |
| 32:QA:1360:A:OP2 | 45:QN:35:ARG:NH2 | 2.42 | 0.52 |
| 32:QA:1479:C:H2' | 32:QA:1480:G:H8 | 1.75 | 0.52 |
| 36:QE:12:LEU:HB3 | 36:QE:31:LEU:HB2 | 1.92 | 0.52 |
| 1:RA:1796:U:H2' | 1:RA:1797:C:C6 | 2.45 | 0.52 |
| 1:YA:1310:G:OP2 | 29:Y7:9:ARG:HD2 | 2.09 | 0.52 |
| 30:Y8:23:VAL:HG13 | 30:Y8:47:LYS:HB3 | 1.92 | 0.52 |
| 1:YA:1019:U:OP1 | 1:YA:1035:U:O2' | 2.23 | 0.52 |
| 32:QA:1479:C:H2' | 32:QA:1480:G:C8 | 2.45 | 0.52 |
| 32:QA:56:U:H2' | 32:QA:57:G:C8 | 2.44 | 0.52 |
| 40:QI:121:ARG:NH1 | 40:QI:122:ALA:O | 2.43 | 0.52 |
| 43:QL:60:LEU:HD21 | 43:QL:66:VAL:HG22 | 1.91 | 0.52 |
| 55:QY:326:LEU:CD1 | 55:QY:328:ARG:HH21 | 2.22 | 0.52 |
| 1:RA:1530:C:HO2' | 1:RA:1531:C:P | 2.32 | 0.52 |
| 1:RA:8:A:H2' | 1:RA:9:U:C6 | 2.44 | 0.52 |
| 13:RR:21:TYR:OH | 13:RR:43:GLU:HG2 | 2.09 | 0.52 |
| 32:XA:539:A:OP2 | 43:XL:115:LYS:NZ | 2.43 | 0.52 |
| 44:XM:19:LEU:HD21 | 44:XM:56:LEU:HD21 | 1.91 | 0.52 |
| 1:YA:1411:C:H2' | 1:YA:1412:A:C8 | 2.45 | 0.52 |
| 1:YA:2602:A:N1 | 55:XY:242:SER:OG | 2.42 | 0.52 |
| 5:YF:157:VAL:HB | 5:YF:194:MET:HG2 | 1.92 | 0.52 |
| 7:YH:115:VAL:HG11 | 7:YH:148:ILE:HD11 | 1.91 | 0.52 |
| 32:QA:1216:G:OP1 | 45:QN:2:ALA:HA | 2.10 | 0.52 |
| 53:QV:9:G:O2' | 53:QV:10:G:N7 | 2.41 | 0.52 |
| 1:RA:2165:G:H2' | 1:RA:2166:G:O4' | 2.09 | 0.52 |
| 18:RW:4:LYS:HG2 | 18:RW:5:ALA:N | 2.24 | 0.52 |
| 32:XA:1391:U:H2' | 32:XA:1392:G:C8 | 2.45 | 0.52 |
| 51:XT:57:ARG:HH12 | 51:XT:100:ILE:HB | 1.75 | 0.52 |
| 1:YA:2165:G:H2' | 1:YA:2166:G:O4' | 2.10 | 0.52 |
| 1:YA:2319:G:H22 | 14:YS:3:ARG:CZ | 2.23 | 0.52 |
| 16:YU:86:ALA:O | 17:YV:49:THR:HG23 | 2.10 | 0.52 |
| 32:QA:1060:C:C5 | 34:QC:2:GLY:HA3 | 2.45 | 0.51 |
| 32:QA:1240:U:C2 | 38:QG:32:ARG:HD3 | 2.45 | 0.51 |
| 35:QD:196:LEU:HD12 | 35:QD:196:LEU:H | 1.76 | 0.51 |
| 1:RA:2284:C:OP1 | 28:R6:5:VAL:HG13 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:RA:1101:U:H2' | 1:RA:1102:C:H6 | 1.75 | 0.51 |
| 1:RA:1991:U:H2' | 1:RA:1992:G:H5'' | 1.91 | 0.51 |
| 1:RA:2099:U:H3 | 1:RA:2190:G:H1 | 1.57 | 0.51 |
| 1:RA:2758:A:C2 | 7:RH:71:LEU:HD21 | 2.45 | 0.51 |
| 21:RZ:129:SER:HB3 | 21:RZ:132:ASN:HB2 | 1.91 | 0.51 |
| 21:RZ:126:VAL:HG11 | 21:RZ:161:VAL:HG23 | 1.92 | 0.51 |
| 32:XA:1218:C:H2' | 32:XA:1219:U:C6 | 2.45 | 0.51 |
| 55:XY:229:SER:OG | 55:XY:242:SER:OG | 2.27 | 0.51 |
| 27:Y5:40:LYS:NZ | 27:Y5:44:THR:O | 2.25 | 0.51 |
| 32:QA:109:A:C6 | 32:QA:326:G:C6 | 2.99 | 0.51 |
| 33:QB:84:GLU:HB3 | 33:QB:219:VAL:HG21 | 1.92 | 0.51 |
| 34:QC:58:GLU:HB3 | 41:QJ:92:THR:HG21 | 1.92 | 0.51 |
| 1:RA:2105:C:N4 | 1:RA:2106:G:O6 | 2.42 | 0.51 |
| 3:RD:106:ILE:O | 3:RD:108:PRO:HD3 | 2.11 | 0.51 |
| 5:RF:101:LEU:O | 5:RF:106:ARG:NH1 | 2.42 | 0.51 |
| 32:XA:1513:A:H2' | 32:XA:1514:C:C6 | 2.45 | 0.51 |
| 55:XY:116:ARG:HH11 | 55:XY:161:GLU:HG3 | 1.75 | 0.51 |
| 22:Y0:8:GLY:N | 53:XV:2:G:H5' | 2.25 | 0.51 |
| 6:YG:56:ALA:HA | 6:YG:153:ARG:NH2 | 2.25 | 0.51 |
| 18:YW:23:LEU:O | 18:YW:27:LYS:NZ | 2.44 | 0.51 |
| 32:QA:164:U:H2' | 32:QA:165:C:C6 | 2.45 | 0.51 |
| 1:RA:833:U:O2 | 11:RP:55:ARG:NH2 | 2.38 | 0.51 |
| 1:RA:878:A:H3' | 1:RA:879:G:H8 | 1.74 | 0.51 |
| 9:RN:62:VAL:CG1 | 9:RN:66:LYS:HB2 | 2.40 | 0.51 |
| 1:RA:956:G:P | 12:RQ:14:ARG:HH22 | 2.33 | 0.51 |
| 19:RX:5:TYR:HB3 | 24:R2:33:MET:HB2 | 1.93 | 0.51 |
| 37:XF:95:GLU:O | 49:XR:32:ARG:NH2 | 2.43 | 0.51 |
| 43:XL:28:LYS:N | 43:XL:29:GLY:HA2 | 2.24 | 0.51 |
| 1:YA:1029:A:H2 | 1:YA:2465:C:H2' | 1.74 | 0.51 |
| 1:YA:218:A:C2 | 1:YA:235:U:H4' | 2.45 | 0.51 |
| 10:YO:2:ILE:HB | 10:YO:33:ALA:HB3 | 1.91 | 0.51 |
| 34:QC:32:LEU:HD22 | 34:QC:59:ARG:NH1 | 2.26 | 0.51 |
| 32:XA:404:U:H5'' | 35:XD:122:ARG:HD3 | 1.90 | 0.51 |
| 32:XA:660:G:H1 | 32:XA:745:C:H42 | 1.58 | 0.51 |
| 33:XB:96:ARG:HD2 | 33:XB:98:LEU:HD23 | 1.91 | 0.51 |
| 34:XC:8:ILE:HD12 | 34:XC:16:ARG:HD3 | 1.93 | 0.51 |
| 32:XA:545:C:OP1 | 35:XD:61:LYS:NZ | 2.44 | 0.51 |
| 44:XM:81:LEU:HD13 | 44:XM:88:ARG:HG2 | 1.92 | 0.51 |
| 47:XP:23:ASP:OD1 | 47:XP:25:ARG:HD3 | 2.10 | 0.51 |
| 1:YA:1721:G:H8 | 1:YA:1741:A:H62 | 1.58 | 0.51 |
| 1:YA:1796:U:H2' | 1:YA:1797:C:C6 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:YF:103:LYS:HA | 5:YF:106:ARG:HD3 | 1.91 | 0.51 |
| 6:YG:97:ASP:HA | 6:YG:100:TRP:HD1 | 1.75 | 0.51 |
| 28:R6:6:ARG:NH1 | 28:R6:26:ASN:HB2 | 2.26 | 0.51 |
| 1:RA:1084:A:H3' | 1:RA:1085:A:H4' | 1.92 | 0.51 |
| 1:RA:1453:U:OP1 | 13:RR:77:ARG:NH1 | 2.39 | 0.51 |
| 1:RA:774:A:H2' | 1:RA:774:A:N3 | 2.26 | 0.51 |
| 21:RZ:92:SER:O | 21:RZ:130:PRO:HG2 | 2.10 | 0.51 |
| 32:XA:1309:G:OP1 | 44:XM:88:ARG:HD2 | 2.09 | 0.51 |
| 32:XA:501:C:H2' | 32:XA:502:G:C8 | 2.45 | 0.51 |
| 35:XD:70:ILE:HD11 | 35:XD:74:GLN:HB3 | 1.93 | 0.51 |
| 36:XE:57:LYS:HG2 | 36:XE:61:TYR:CE2 | 2.44 | 0.51 |
| 46:XO:39:LEU:HD13 | 46:XO:56:LEU:HB2 | 1.92 | 0.51 |
| 1:YA:2573:C:H41 | 55:XY:239:THR:HA | 1.72 | 0.51 |
| 23:Y1:3:LYS:HB2 | 23:Y1:61:ARG:NH1 | 2.26 | 0.51 |
| 1:YA:250:G:P | 30:Y8:13:ARG:HH22 | 2.33 | 0.51 |
| 1:YA:2168:G:H22 | 1:YA:2171:A:H2' | 1.75 | 0.51 |
| 32:QA:1402:4OC:HM22 | 32:QA:1403:C:H5' | 1.92 | 0.51 |
| 34:QC:179:ARG:NH1 | 34:QC:206:GLU:OE1 | 2.44 | 0.51 |
| 41:QJ:38:ILE:HG12 | 41:QJ:71:LEU:HB3 | 1.91 | 0.51 |
| 1:RA:1756:G:H4' | 1:RA:1758:G:O4' | 2.11 | 0.51 |
| 1:RA:587:C:P | 11:RP:21:ARG:HH22 | 2.34 | 0.51 |
| 4:RE:105:THR:OG1 | 4:RE:199:ARG:NH2 | 2.44 | 0.51 |
| 20:RY:13:VAL:HB | 20:RY:72:VAL:HG13 | 1.93 | 0.51 |
| 32:XA:1346:A:OP1 | 40:XI:120:ARG:NH1 | 2.38 | 0.51 |
| 32:XA:841:U:C5 | 32:XA:848:C:H1' | 2.46 | 0.51 |
| 32:XA:858:G:O6 | 32:XA:869:G:H3' | 2.11 | 0.51 |
| 36:XE:6:PHE:HB2 | 36:XE:34:VAL:HG13 | 1.91 | 0.51 |
| 1:YA:1069:A:H5' | 1:YA:1096:A:H5' | 1.93 | 0.51 |
| 1:YA:273(A):G:H4' | 1:YA:273(B):U:H5'' | 1.91 | 0.51 |
| 6:YG:5:VAL:HG12 | 26:Y4:25:TYR:CE1 | 2.45 | 0.51 |
| 32:QA:1101:A:H4' | 32:QA:1102:A:O5' | 2.10 | 0.51 |
| 32:QA:1278:U:H5'' | 32:QA:1279:A:H5' | 1.92 | 0.51 |
| 32:QA:946:A:H2' | 32:QA:947:G:C8 | 2.46 | 0.51 |
| 35:QD:108:LEU:HB3 | 35:QD:110:PHE:CE1 | 2.46 | 0.51 |
| 50:QS:41:VAL:HG22 | 50:QS:42:PRO:HD2 | 1.93 | 0.51 |
| 28:R6:13:CYS:SG | 28:R6:47:THR:HG21 | 2.51 | 0.51 |
| 1:RA:1019:U:OP1 | 1:RA:1035:U:O2' | 2.23 | 0.51 |
| 1:RA:2698:U:H2' | 1:RA:2699:C:C6 | 2.46 | 0.51 |
| 36:XE:144:THR:H | 36:XE:147:ASP:HB2 | 1.76 | 0.51 |
| 32:XA:229:U:O2' | 47:XP:23:ASP:OD2 | 2.28 | 0.51 |
| 1:YA:2134:A:H8 | 1:YA:2156:G:H21 | 1.59 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:YA:2683:C:OP1 | 15:YT:53:ARG:NH2 | 2.44 | 0.51 |
| 7:YH:55:PRO:HG2 | 7:YH:61:HIS:CE1 | 2.45 | 0.51 |
| 20:YY:38:ILE:HD11 | 20:YY:66:PRO:HG3 | 1.92 | 0.51 |
| 38:QG:111:ARG:NH1 | 38:QG:113:GLU:OE1 | 2.43 | 0.51 |
| 32:XA:1304:G:OP1 | 52:XU:2:GLY:N | 2.43 | 0.51 |
| 32:XA:926:G:H22 | 54:XX:16:A:P | 2.33 | 0.51 |
| 55:XY:316:ARG:NH2 | 55:XY:327:TYR:OH | 2.43 | 0.51 |
| 26:Y4:15:ILE:HD12 | 26:Y4:21:VAL:HG22 | 1.93 | 0.51 |
| 1:YA:2206:G:H8 | 1:YA:2207:G:N7 | 2.09 | 0.51 |
| 1:YA:2698:U:H2' | 1:YA:2699:C:C6 | 2.45 | 0.51 |
| 32:QA:1227:A:OP1 | 50:QS:80:TYR:OH | 2.24 | 0.51 |
| 32:QA:189(L):U:H2' | 32:QA:189(M):G:H8 | 1.76 | 0.51 |
| 32:QA:189(L):U:H2' | 32:QA:189(M):G:C8 | 2.46 | 0.51 |
| 30:R8:62:LEU:HB3 | 30:R8:65:GLU:HG2 | 1.92 | 0.51 |
| 1:RA:1053:C:O2' | 1:RA:1054:A:O4' | 2.27 | 0.51 |
| 8:RI:133:HIS:ND1 | 8:RI:134:PRO:O | 2.44 | 0.51 |
| 1:YA:61:G:H5' | 24:Y2:50:ILE:HG21 | 1.93 | 0.51 |
| 1:YA:1778:U:H2' | 1:YA:1784:A:N6 | 2.26 | 0.51 |
| 1:YA:2023:G:H5' | 1:YA:2617:C:H4' | 1.93 | 0.51 |
| 32:QA:186:C:H2' | 32:QA:187:C:C6 | 2.45 | 0.51 |
| 41:QJ:37:PRO:HA | 41:QJ:72:VAL:HG12 | 1.92 | 0.51 |
| 1:RA:954:G:O2' | 1:RA:2274:A:N1 | 2.40 | 0.51 |
| 1:RA:2334:G:H5' | 14:RS:9:ARG:HG2 | 1.93 | 0.51 |
| 6:RG:50:ALA:O | 6:RG:52:ILE:N | 2.44 | 0.51 |
| 12:RQ:14:ARG:HG2 | 12:RQ:41:TRP:HH2 | 1.76 | 0.51 |
| 19:RX:60:ARG:HH22 | 29:R7:47:ARG:HH22 | 1.57 | 0.51 |
| 32:XA:1118:C:H1' | 32:XA:1179:A:C4 | 2.46 | 0.51 |
| 1:YA:1593:G:H2' | 1:YA:1594:G:C8 | 2.46 | 0.51 |
| 1:YA:489:G:N7 | 18:YW:49:LYS:NZ | 2.58 | 0.51 |
| 7:YH:28:GLY:HA3 | 7:YH:79:VAL:HB | 1.92 | 0.51 |
| 32:QA:368:U:O4 | 8:YI:82:ARG:HD2 | 2.11 | 0.51 |
| 1:YA:300:A:OP1 | 20:YY:86:ARG:NH2 | 2.44 | 0.51 |
| 32:QA:1347:G:H5' | 40:QI:107:ARG:HB3 | 1.93 | 0.50 |
| 32:QA:1510:U:H2' | 32:QA:1511:G:C8 | 2.45 | 0.50 |
| 32:QA:881:G:P | 43:QL:12:ARG:HH22 | 2.33 | 0.50 |
| 53:QV:51:C:H2' | 53:QV:52:G:O4' | 2.11 | 0.50 |
| 1:RA:321:G:H5' | 5:RF:134:GLY:O | 2.10 | 0.50 |
| 1:RA:784:A:C6 | 3:RD:229:VAL:HG11 | 2.45 | 0.50 |
| 5:RF:12:LEU:HD13 | 5:RF:124:LEU:HD11 | 1.93 | 0.50 |
| 32:XA:921:U:O2' | 36:XE:19:MET:O | 2.19 | 0.50 |
| 1:YA:1932:A:H2' | 1:YA:1933:G:O4' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:YG:66:GLN:HB3 | 6:YG:92:VAL:HG21 | 1.91 | 0.50 |
| 32:QA:441:A:H3' | 32:QA:442:C:C6 | 2.45 | 0.50 |
| 32:QA:973:G:H3' | 32:QA:974:A:H5'' | 1.93 | 0.50 |
| 1:RA:1667:G:O2' | 1:RA:1991:U:O4 | 2.23 | 0.50 |
| 32:XA:689:C:OP1 | 42:XK:27:ASN:ND2 | 2.38 | 0.50 |
| 47:XP:20:VAL:HG21 | 47:XP:32:TYR:CG | 2.46 | 0.50 |
| 30:Y8:23:VAL:HG11 | 30:Y8:47:LYS:HD3 | 1.93 | 0.50 |
| 1:YA:616:G:H5' | 5:YF:205:ARG:HD2 | 1.93 | 0.50 |
| 11:YP:100:LEU:HD22 | 11:YP:105:LEU:HD12 | 1.91 | 0.50 |
| 32:QA:171:A:H2' | 32:QA:172:A:C8 | 2.47 | 0.50 |
| 32:QA:454:C:OP2 | 32:QA:455:C:N4 | 2.39 | 0.50 |
| 32:QA:629:G:H2' | 32:QA:630:G:O4' | 2.11 | 0.50 |
| 44:QM:19:LEU:HD21 | 44:QM:56:LEU:HD21 | 1.93 | 0.50 |
| 30:R8:23:VAL:HG11 | 30:R8:47:LYS:HD3 | 1.92 | 0.50 |
| 1:RA:272(L):U:H5' | 8:RI:50:ARG:NH1 | 2.26 | 0.50 |
| 11:RP:99:LEU:HD23 | 11:RP:102:ARG:HH21 | 1.77 | 0.50 |
| 32:XA:1146:A:H3' | 32:XA:1147:C:H5'' | 1.92 | 0.50 |
| 32:XA:380:G:N2 | 32:XA:383:A:OP2 | 2.44 | 0.50 |
| 33:XB:95:GLN:HG3 | 33:XB:147:LYS:O | 2.11 | 0.50 |
| 12:YQ:80:GLU:CD | 55:XY:264:HIS:HB2 | 2.32 | 0.50 |
| 6:YG:120:LEU:HB3 | 6:YG:131:TYR:OH | 2.11 | 0.50 |
| 32:QA:1305:G:N2 | 32:QA:1331:G:H1' | 2.26 | 0.50 |
| 32:QA:67:C:H2' | 32:QA:68:G:C8 | 2.47 | 0.50 |
| 32:QA:96:U:H2' | 32:QA:97:G:C8 | 2.45 | 0.50 |
| 33:QB:178:ARG:NH2 | 39:QH:68:ARG:HH12 | 2.09 | 0.50 |
| 27:R5:16:ARG:HH11 | 27:R5:16:ARG:HG2 | 1.76 | 0.50 |
| 1:RA:2206:G:H5'' | 1:RA:2207:G:N7 | 2.25 | 0.50 |
| 1:RA:2345:G:H1' | 1:RA:2382:G:H5' | 1.93 | 0.50 |
| 32:XA:1005:A:H5'' | 32:XA:1006:C:C5 | 2.46 | 0.50 |
| 35:XD:162:LEU:HD13 | 35:XD:181:MET:HG2 | 1.93 | 0.50 |
| 42:XK:115:PRO:C | 42:XK:117:ASN:HA | 2.31 | 0.50 |
| 51:XT:18:GLN:O | 51:XT:22:ARG:HG3 | 2.10 | 0.50 |
| 1:YA:2115:G:N1 | 1:YA:2117:A:N7 | 2.58 | 0.50 |
| 1:YA:2180:U:H2' | 1:YA:2181:G:C8 | 2.45 | 0.50 |
| 2:YB:66:A:H61 | 2:YB:109:C:H5' | 1.76 | 0.50 |
| 1:YA:997:G:OP1 | 16:YU:92:ARG:HG2 | 2.11 | 0.50 |
| 38:QG:48:LYS:O | 38:QG:52:GLU:HG2 | 2.12 | 0.50 |
| 1:RA:1794:U:H2' | 1:RA:1795:C:C6 | 2.47 | 0.50 |
| 1:RA:2104:G:N2 | 1:RA:2105:C:C4 | 2.80 | 0.50 |
| 32:XA:1100:C:H2' | 32:XA:1102:A:O5' | 2.11 | 0.50 |
| 45:YN:32:SER:OG | 45:YN:41:ARG:HG2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:1058:G:H1 | 1:YA:1080:C:H42 | 1.60 | 0.50 |
| 1:YA:1063:G:H2' | 1:YA:1065:U:H6 | 1.76 | 0.50 |
| 32:QA:838:G:H2' | 32:QA:839:U:H2' | 1.93 | 0.50 |
| 40:QI:16:ARG:HB2 | 40:QI:64:THR:HG22 | 1.94 | 0.50 |
| 55:QY:328:ARG:HD2 | 55:QY:332:VAL:HG23 | 1.93 | 0.50 |
| 1:RA:1068:G:H3' | 1:RA:1096:A:OP2 | 2.12 | 0.50 |
| 1:RA:2785:C:O2' | 4:RE:66:HIS:ND1 | 2.38 | 0.50 |
| 33:XB:201:ILE:HG21 | 33:XB:214:ILE:HG21 | 1.93 | 0.50 |
| 47:XP:59:TRP:HA | 47:XP:62:VAL:HG12 | 1.94 | 0.50 |
| 32:XA:1313:U:P | 50:XS:5:LEU:HG | 2.51 | 0.50 |
| 25:Y3:23:LEU:HD22 | 25:Y3:50:VAL:HG11 | 1.93 | 0.50 |
| 1:YA:1364:G:OP2 | 23:Y1:3:LYS:HG3 | 2.11 | 0.50 |
| 6:YG:3:LEU:H | 6:YG:3:LEU:HD23 | 1.76 | 0.50 |
| 7:YH:87:LEU:HD23 | 7:YH:164:TYR:HA | 1.93 | 0.50 |
| 9:YN:96:GLU:HB2 | 9:YN:122:VAL:HG12 | 1.93 | 0.50 |
| 1:RA:1223:G:N2 | 1:RA:1226:A:OP2 | 2.39 | 0.50 |
| 16:RU:76:TYR:CZ | 16:RU:80:ILE:HG13 | 2.46 | 0.50 |
| 32:XA:1302:U:OP2 | 44:XM:21:TYR:OH | 2.22 | 0.50 |
| 32:XA:429:U:H3' | 35:XD:9:CYS:SG | 2.52 | 0.50 |
| 32:XA:1456:G:N1 | 51:XT:51:GLU:OE1 | 2.44 | 0.50 |
| 5:YF:21:ALA:HB3 | 5:YF:22:ALA:HA | 1.94 | 0.50 |
| 1:RA:2168:G:H22 | 1:RA:2171:A:H2' | 1.77 | 0.50 |
| 26:Y4:20:ASN:HD21 | 26:Y4:38:LYS:HG3 | 1.76 | 0.50 |
| 27:Y5:16:ARG:HH11 | 27:Y5:16:ARG:HG2 | 1.77 | 0.50 |
| 1:YA:26:G:C6 | 1:YA:27:G:N1 | 2.79 | 0.50 |
| 14:YS:67:ARG:HG3 | 14:YS:71:ARG:NH1 | 2.27 | 0.50 |
| 1:YA:583:G:OP2 | 16:YU:10:ARG:HD2 | 2.12 | 0.50 |
| 16:YU:76:TYR:OH | 16:YU:92:ARG:NH1 | 2.44 | 0.50 |
| 33:QB:115:LEU:HD13 | 33:QB:145:LEU:HB3 | 1.93 | 0.50 |
| 50:QS:50:ALA:HB1 | 50:QS:57:HIS:HB3 | 1.93 | 0.50 |
| 51:QT:10:LEU:HD23 | 51:QT:11:SER:H | 1.77 | 0.50 |
| 1:RA:2704:C:H2' | 1:RA:2705:A:O4' | 2.11 | 0.50 |
| 1:RA:642:G:N2 | 1:RA:645:C:OP2 | 2.45 | 0.50 |
| 1:RA:796:C:H2' | 1:RA:797:C:C6 | 2.47 | 0.50 |
| 8:RI:140:LEU:HD12 | 8:RI:142:VAL:HG22 | 1.93 | 0.50 |
| 32:XA:1376:U:H2' | 32:XA:1377:A:C8 | 2.47 | 0.50 |
| 32:XA:881:G:P | 43:XL:12:ARG:HH22 | 2.35 | 0.50 |
| 34:XC:152:ILE:HG22 | 34:XC:167:TRP:HB2 | 1.94 | 0.50 |
| 1:YA:1739:U:HO2' | 1:YA:1740:G:H8 | 1.58 | 0.50 |
| 1:YA:514:A:N3 | 1:YA:581:C:O2' | 2.43 | 0.50 |
| 1:YA:642:G:N2 | 1:YA:645:C:OP2 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:YA:1812:A:O2' | 3:YD:45:ASN:N | 2.45 | 0.50 |
| 4:YE:51:PHE:O | 4:YE:77:ILE:N | 2.44 | 0.50 |
| 32:QA:1030(D):G:H2' | 32:QA:1030(E):A:C8 | 2.46 | 0.49 |
| 32:QA:1157:A:H4' | 32:QA:1158:C:O5' | 2.12 | 0.49 |
| 32:QA:509:A:N3 | 32:QA:543:C:O2' | 2.39 | 0.49 |
| 34:QC:70:VAL:HG22 | 34:QC:72:LYS:H | 1.77 | 0.49 |
| 26:R4:16:CYS:SG | 26:R4:17:GLY:N | 2.85 | 0.49 |
| 1:RA:2420:C:H5'' | 28:R6:8:LYS:HD2 | 1.94 | 0.49 |
| 1:RA:265:A:N1 | 1:RA:427:U:O2' | 2.38 | 0.49 |
| 1:RA:479:A:N3 | 1:RA:481:G:H5'' | 2.27 | 0.49 |
| 6:RG:77:ILE:HG13 | 6:RG:82:LEU:HD12 | 1.94 | 0.49 |
| 26:Y4:15:ILE:HB | 26:Y4:32:TYR:CD1 | 2.47 | 0.49 |
| 1:YA:1794:U:H2' | 1:YA:1795:C:C6 | 2.47 | 0.49 |
| 1:YA:2805:G:H2' | 1:YA:2807:G:H8 | 1.77 | 0.49 |
| 6:YG:7:LEU:HD23 | 6:YG:100:TRP:HE3 | 1.76 | 0.49 |
| 9:YN:54:VAL:HB | 9:YN:122:VAL:HG22 | 1.94 | 0.49 |
| 14:YS:14:VAL:O | 14:YS:18:ILE:HG12 | 2.11 | 0.49 |
| 32:QA:1356:G:H2' | 32:QA:1357:A:C8 | 2.47 | 0.49 |
| 55:QY:138:TYR:HD1 | 55:QY:336:LYS:HB2 | 1.77 | 0.49 |
| 32:XA:1179:A:H2' | 32:XA:1180:A:O4' | 2.12 | 0.49 |
| 33:XB:16:HIS:CD2 | 33:XB:210:SER:HB3 | 2.48 | 0.49 |
| 34:XC:22:TRP:CD1 | 34:XC:59:ARG:HD2 | 2.48 | 0.49 |
| 55:XY:138:TYR:HD1 | 55:XY:336:LYS:HB2 | 1.77 | 0.49 |
| 1:YA:2233:U:H2' | 1:YA:2234:G:C8 | 2.47 | 0.49 |
| 1:YA:572:A:OP2 | 17:YV:78:LYS:NZ | 2.39 | 0.49 |
| 32:QA:1255:G:OP1 | 41:QJ:45:ARG:NH2 | 2.43 | 0.49 |
| 1:RA:9:U:O2' | 1:RA:10:G:OP1 | 2.30 | 0.49 |
| 9:RN:94:HIS:CB | 9:RN:97:ARG:HD3 | 2.42 | 0.49 |
| 32:XA:1030(A):C:H42 | 32:XA:1031:G:H1 | 1.58 | 0.49 |
| 32:XA:1270:C:O2' | 32:XA:1314:C:H5' | 2.11 | 0.49 |
| 40:XI:5:TYR:HE1 | 40:XI:16:ARG:HB3 | 1.77 | 0.49 |
| 42:XK:84:VAL:HG21 | 42:XK:95:ILE:HD11 | 1.94 | 0.49 |
| 32:XA:1340:A:O2' | 53:XV:32:C:H5' | 2.12 | 0.49 |
| 1:YA:272(E):U:H2' | 1:YA:272(F):C:C6 | 2.47 | 0.49 |
| 1:YA:910:A:N1 | 1:YA:2277:G:H1' | 2.28 | 0.49 |
| 32:QA:1003:G:C2' | 32:QA:1004:A:H4' | 2.42 | 0.49 |
| 32:QA:1118:C:H1' | 32:QA:1179:A:C4 | 2.47 | 0.49 |
| 33:QB:178:ARG:HH22 | 39:QH:68:ARG:NH1 | 2.10 | 0.49 |
| 39:QH:14:ARG:O | 39:QH:18:ARG:HG2 | 2.12 | 0.49 |
| 26:R4:57:GLU:HB2 | 26:R4:58:ARG:HA | 1.93 | 0.49 |
| 1:RA:26:G:C6 | 1:RA:27:G:N1 | 2.80 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:RH:4:ILE:O | 7:RH:69:ARG:HG2 | 2.12 | 0.49 |
| 15:RT:28:VAL:HG13 | 15:RT:86:ILE:HG23 | 1.94 | 0.49 |
| 16:RU:61:TRP:CH2 | 16:RU:93:LYS:HB2 | 2.48 | 0.49 |
| 40:XI:5:TYR:OH | 40:XI:16:ARG:HG2 | 2.12 | 0.49 |
| 1:YA:824:A:H1' | 1:YA:2358:G:N7 | 2.28 | 0.49 |
| 1:YA:300:A:H1' | 1:YA:319:C:H1' | 1.94 | 0.49 |
| 6:YG:146:TYR:HD2 | 44:XM:8:GLU:CD | 2.14 | 0.49 |
| 55:QY:101:LEU:H | 55:QY:102:PRO:HD2 | 1.76 | 0.49 |
| 26:R4:44:THR:O | 26:R4:46:GLN:N | 2.46 | 0.49 |
| 1:RA:2285:C:H5'' | 28:R6:29:ASN:ND2 | 2.27 | 0.49 |
| 1:RA:2031:A:C6 | 1:RA:2498:C:H1' | 2.48 | 0.49 |
| 5:RF:184:TYR:O | 5:RF:188:ARG:HG3 | 2.12 | 0.49 |
| 7:RH:25:LYS:HG3 | 7:RH:34:GLU:HG2 | 1.93 | 0.49 |
| 32:XA:1002:G:N3 | 32:XA:1003:G:C8 | 2.81 | 0.49 |
| 36:XE:33:VAL:HG21 | 36:XE:109:ILE:HA | 1.95 | 0.49 |
| 1:YA:2130:U:H2' | 1:YA:2158:A:H61 | 1.77 | 0.49 |
| 1:YA:8:A:H2' | 1:YA:9:U:C6 | 2.48 | 0.49 |
| 1:YA:764:A:H5' | 3:YD:210:GLY:HA2 | 1.95 | 0.49 |
| 14:YS:93:LYS:HD2 | 14:YS:95:HIS:HB2 | 1.93 | 0.49 |
| 32:QA:555:C:H2' | 32:QA:556:C:C6 | 2.48 | 0.49 |
| 26:R4:54:GLY:O | 26:R4:56:VAL:HA | 2.12 | 0.49 |
| 33:XB:9:GLU:C | 33:XB:11:LEU:H | 2.15 | 0.49 |
| 33:XB:124:SER:HB2 | 33:XB:125:PRO:HD3 | 1.94 | 0.49 |
| 36:XE:143:ARG:NH1 | 39:XH:77:GLU:OE2 | 2.42 | 0.49 |
| 1:YA:1028:A:O2' | 1:YA:1029:A:O4' | 2.30 | 0.49 |
| 1:YA:1057:A:HO2' | 1:YA:1058:G:P | 2.34 | 0.49 |
| 1:YA:1063:G:H2' | 1:YA:1065:U:C6 | 2.47 | 0.49 |
| 1:YA:1411:C:H2' | 1:YA:1412:A:H8 | 1.77 | 0.49 |
| 1:YA:1889:A:H2' | 1:YA:1890:A:C8 | 2.48 | 0.49 |
| 1:YA:2389:G:H5'' | 1:YA:2390:U:O4' | 2.12 | 0.49 |
| 7:YH:90:LYS:HD2 | 7:YH:163:TYR:CD1 | 2.48 | 0.49 |
| 11:YP:50:ARG:HD3 | 30:Y8:7:HIS:CD2 | 2.47 | 0.49 |
| 32:QA:1060:C:C4 | 34:QC:2:GLY:HA3 | 2.47 | 0.49 |
| 32:QA:950:U:OP2 | 44:QM:102:ARG:HD2 | 2.13 | 0.49 |
| 49:QR:47:THR:HG23 | 49:QR:49:LYS:HG3 | 1.94 | 0.49 |
| 55:QY:204:ALA:HB2 | 55:QY:298:LEU:HD21 | 1.94 | 0.49 |
| 23:R1:51:VAL:HG12 | 23:R1:53:VAL:HG23 | 1.95 | 0.49 |
| 1:RA:1101:U:H2' | 1:RA:1102:C:C6 | 2.48 | 0.49 |
| 1:RA:2074:U:H2' | 1:RA:2075:U:C6 | 2.47 | 0.49 |
| 1:RA:272(K):U:H1' | 8:RI:50:ARG:NH2 | 2.22 | 0.49 |
| 1:RA:2805:G:H2' | 1:RA:2807:G:C8 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:XA:978:A:O2' | 32:XA:1322:C:N3 | 2.37 | 0.49 |
| 38:XG:45:ASP:O | 38:XG:49:ILE:HG13 | 2.11 | 0.49 |
| 1:YA:1923:U:OP1 | 53:XV:24:U:O2' | 2.29 | 0.49 |
| 11:YP:63:PRO:HD3 | 30:Y8:27:THR:HG22 | 1.94 | 0.49 |
| 1:YA:1607:C:N4 | 1:YA:1622:G:OP2 | 2.31 | 0.49 |
| 5:YF:110:LEU:HA | 5:YF:183:VAL:HG12 | 1.95 | 0.49 |
| 15:YT:64:ARG:HB2 | 15:YT:73:GLU:HG2 | 1.95 | 0.49 |
| 32:QA:1513:A:H2' | 32:QA:1514:C:C6 | 2.48 | 0.49 |
| 32:QA:235:C:H5' | 48:QQ:70:ARG:HG2 | 1.93 | 0.49 |
| 32:QA:1106:G:H5' | 34:QC:172:ARG:HG2 | 1.94 | 0.49 |
| 34:QC:47:LEU:HD13 | 34:QC:68:VAL:HG11 | 1.93 | 0.49 |
| 48:QQ:6:LEU:HG | 48:QQ:23:VAL:HG11 | 1.94 | 0.49 |
| 1:RA:1065:U:H4' | 1:RA:1066:U:H5' | 1.94 | 0.49 |
| 1:RA:1224:C:O2' | 17:RV:85:LYS:HA | 2.13 | 0.49 |
| 1:RA:1721:G:H8 | 1:RA:1741:A:H62 | 1.60 | 0.49 |
| 1:RA:323:G:C8 | 5:RF:171:PRO:HG3 | 2.47 | 0.49 |
| 1:RA:468:G:N7 | 29:R7:39:ARG:NH2 | 2.53 | 0.49 |
| 7:RH:3:ARG:HH22 | 7:RH:66:GLY:HA3 | 1.77 | 0.49 |
| 32:XA:512:U:H2' | 32:XA:513:C:C6 | 2.48 | 0.49 |
| 32:XA:70:G:H1 | 32:XA:99:U:H3 | 1.61 | 0.49 |
| 34:XC:152:ILE:CG1 | 34:XC:199:LYS:HB2 | 2.43 | 0.49 |
| 34:XC:32:LEU:HD12 | 34:XC:59:ARG:NH1 | 2.28 | 0.49 |
| 32:XA:406:G:O2' | 35:XD:3:ARG:NH2 | 2.46 | 0.49 |
| 37:XF:67:MET:SD | 37:XF:72:VAL:HG12 | 2.53 | 0.49 |
| 49:XR:47:THR:HG23 | 49:XR:49:LYS:HG3 | 1.93 | 0.49 |
| 50:XS:20:LEU:HD23 | 50:XS:23:ASN:ND2 | 2.24 | 0.49 |
| 26:Y4:57:GLU:CB | 26:Y4:58:ARG:HD2 | 2.42 | 0.49 |
| 1:YA:2105:C:N4 | 1:YA:2106:G:O6 | 2.46 | 0.49 |
| 1:YA:2298:A:H62 | 1:YA:2318:G:H8 | 1.60 | 0.49 |
| 9:YN:46:VAL:HG23 | 9:YN:48:MET:HG2 | 1.94 | 0.49 |
| 51:QT:57:ARG:HH22 | 51:QT:100:ILE:HD12 | 1.78 | 0.49 |
| 28:R6:6:ARG:NE | 28:R6:24:GLU:OE1 | 2.32 | 0.49 |
| 30:R8:23:VAL:HG13 | 30:R8:47:LYS:HB3 | 1.94 | 0.49 |
| 1:RA:1032:A:H1' | 31:R9:23:VAL:HG21 | 1.94 | 0.49 |
| 1:RA:362:U:O2' | 1:RA:363(A):G:H5' | 2.12 | 0.49 |
| 4:RE:51:PHE:H | 4:RE:75:VAL:HG11 | 1.77 | 0.49 |
| 1:RA:1188:U:H4' | 17:RV:79:VAL:HG22 | 1.95 | 0.49 |
| 32:XA:1135:U:H2' | 32:XA:1137:C:N3 | 2.28 | 0.49 |
| 32:XA:1223:C:P | 50:XS:78:ARG:HH22 | 2.36 | 0.49 |
| 32:XA:1366:C:O2' | 41:XJ:60:ARG:NH2 | 2.31 | 0.49 |
| 32:XA:328:C:H4' | 32:XA:329:A:H5' | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 36:XE:137:GLU:OE1 | 36:XE:141:GLN:NE2 | 2.40 | 0.49 |
| 1:YA:2243:U:H2' | 1:YA:2244:U:C6 | 2.47 | 0.49 |
| 6:YG:41:GLN:NE2 | 6:YG:154:GLY:O | 2.40 | 0.49 |
| 32:QA:1010:G:H22 | 32:QA:1020:U:H1' | 1.78 | 0.49 |
| 32:QA:1062:U:H2' | 32:QA:1063:C:C6 | 2.47 | 0.49 |
| 34:QC:58:GLU:O | 34:QC:64:VAL:HG23 | 2.13 | 0.49 |
| 27:R5:45:VAL:HG11 | 27:R5:58:LEU:HD12 | 1.93 | 0.49 |
| 1:RA:1059:G:N1 | 1:RA:1079:C:N4 | 2.61 | 0.49 |
| 1:RA:2115:G:N1 | 1:RA:2117:A:N7 | 2.61 | 0.49 |
| 3:RD:108:PRO:HG3 | 3:RD:143:HIS:CE1 | 2.48 | 0.49 |
| 21:RZ:182:LYS:O | 21:RZ:185:GLU:HG3 | 2.13 | 0.49 |
| 36:XE:92:LYS:HB3 | 36:XE:119:LEU:HB2 | 1.95 | 0.49 |
| 40:XI:23:ASN:H | 40:XI:23:ASN:HD22 | 1.60 | 0.49 |
| 1:YA:881:G:H2' | 1:YA:882:G:C8 | 2.47 | 0.49 |
| 32:QA:1151:A:O2' | 32:QA:1152:A:H8 | 1.96 | 0.48 |
| 32:QA:632:A:H5' | 32:QA:633:G:OP2 | 2.12 | 0.48 |
| 45:QN:48:ALA:HB2 | 45:QN:53:LEU:HD12 | 1.95 | 0.48 |
| 46:QO:16:ALA:HB1 | 46:QO:21:ASP:HB3 | 1.95 | 0.48 |
| 30:R8:14:VAL:HG13 | 30:R8:22:VAL:HG13 | 1.95 | 0.48 |
| 1:RA:1084:A:C8 | 1:RA:1085:A:H4' | 2.48 | 0.48 |
| 1:RA:1803:A:H4' | 3:RD:259:THR:HG23 | 1.95 | 0.48 |
| 6:RG:77:ILE:N | 6:RG:82:LEU:O | 2.37 | 0.48 |
| 32:XA:1030(D):G:H2' | 32:XA:1030(E):A:C8 | 2.48 | 0.48 |
| 47:XP:68:ASP:O | 47:XP:71:ARG:HG2 | 2.13 | 0.48 |
| 1:YA:1104:C:H2' | 1:YA:1105:U:C6 | 2.48 | 0.48 |
| 1:YA:2137:C:C2 | 1:YA:2154:G:N1 | 2.81 | 0.48 |
| 1:YA:2391:G:O6 | 1:YA:2425:A:H8 | 1.96 | 0.48 |
| 1:YA:994:C:OP1 | 16:YU:53:ARG:NH2 | 2.46 | 0.48 |
| 32:QA:103:C:O2' | 32:QA:172:A:N1 | 2.32 | 0.48 |
| 32:QA:341:C:H2' | 32:QA:342:C:C6 | 2.48 | 0.48 |
| 33:QB:166:ASP:OD2 | 33:QB:169:LYS:HB2 | 2.13 | 0.48 |
| 32:QA:532:A:N6 | 34:QC:193:TYR:HA | 2.23 | 0.48 |
| 41:QJ:78:ASN:O | 41:QJ:80:LYS:N | 2.46 | 0.48 |
| 1:RA:2689:U:P | 1:RA:2719:G:H22 | 2.36 | 0.48 |
| 33:XB:16:HIS:O | 33:XB:18:GLY:N | 2.46 | 0.48 |
| 34:XC:36:ASP:O | 34:XC:40:ARG:HG3 | 2.13 | 0.48 |
| 35:XD:108:LEU:HB3 | 35:XD:110:PHE:CE1 | 2.48 | 0.48 |
| 40:XI:16:ARG:HD3 | 40:XI:64:THR:HG21 | 1.93 | 0.48 |
| 30:Y8:46:ARG:HB2 | 30:Y8:46:ARG:HH21 | 1.78 | 0.48 |
| 1:YA:1059:G:N1 | 1:YA:1079:C:N4 | 2.61 | 0.48 |
| 1:YA:2104:G:O6 | 1:YA:2186:G:C4 | 2.66 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:YP:101:VAL:HA | 11:YP:106:LEU:O | 2.14 | 0.48 |
| 32:QA:1070:U:H2' | 32:QA:1071:C:C6 | 2.47 | 0.48 |
| 32:QA:524:G:H2' | 32:QA:525:C:C6 | 2.48 | 0.48 |
| 32:QA:542:G:H5' | 35:QD:41:GLY:HA3 | 1.94 | 0.48 |
| 50:QS:3:ARG:HH21 | 50:QS:7:LYS:HE2 | 1.77 | 0.48 |
| 1:RA:2343:C:O2' | 1:RA:2373:G:O2' | 2.10 | 0.48 |
| 1:RA:2390:U:P | 30:R8:35:GLN:HE22 | 2.36 | 0.48 |
| 33:XB:155:LEU:HD21 | 33:XB:159:PRO:HG3 | 1.95 | 0.48 |
| 36:XE:122:GLU:O | 36:XE:126:ARG:NH1 | 2.46 | 0.48 |
| 43:XL:77:LEU:HD21 | 43:XL:107:ALA:HA | 1.96 | 0.48 |
| 49:XR:52:PRO:HB2 | 49:XR:54:ARG:HG2 | 1.95 | 0.48 |
| 53:XV:50:U:H3 | 53:XV:64:G:H1 | 1.61 | 0.48 |
| 1:YA:1084:A:H3' | 1:YA:1085:A:C4' | 2.44 | 0.48 |
| 1:YA:1525:G:H2' | 1:YA:1526:G:C8 | 2.47 | 0.48 |
| 5:YF:165:ARG:HG2 | 5:YF:168:ARG:NH2 | 2.28 | 0.48 |
| 9:YN:94:HIS:CB | 9:YN:97:ARG:HD3 | 2.42 | 0.48 |
| 32:QA:1023:G:H2' | 32:QA:1024:G:C8 | 2.48 | 0.48 |
| 6:RG:101:ILE:HD13 | 26:R4:25:TYR:HB2 | 1.94 | 0.48 |
| 1:RA:1341:U:OP1 | 1:RA:1397:U:N3 | 2.37 | 0.48 |
| 1:RA:2537:U:H2' | 1:RA:2538:C:C6 | 2.49 | 0.48 |
| 1:RA:330:A:N7 | 1:RA:1210:A:O2' | 2.33 | 0.48 |
| 8:RI:130:TYR:CE2 | 8:RI:132:PRO:HB3 | 2.49 | 0.48 |
| 32:XA:222:U:H2' | 32:XA:223:U:C6 | 2.48 | 0.48 |
| 32:XA:973:G:H3' | 32:XA:974:A:H5" | 1.94 | 0.48 |
| 11:YP:62:LEU:O | 30:Y8:13:ARG:HD3 | 2.13 | 0.48 |
| 6:YG:67:LYS:HE3 | 6:YG:68:PRO:O | 2.13 | 0.48 |
| 32:QA:1202:G:N1 | 45:QN:46:GLU:OE1 | 2.46 | 0.48 |
| 32:QA:1377:A:HO2' | 38:QG:2:ALA:N | 2.11 | 0.48 |
| 32:QA:769:G:H4' | 32:QA:1513:A:H4' | 1.96 | 0.48 |
| 33:QB:15:VAL:O | 33:QB:15:VAL:HG22 | 2.14 | 0.48 |
| 35:QD:108:LEU:HD21 | 35:QD:174:LEU:HD22 | 1.95 | 0.48 |
| 41:QJ:40:LEU:HB2 | 41:QJ:69:ASN:HB2 | 1.95 | 0.48 |
| 44:QM:3:ARG:O | 44:QM:57:ARG:NH2 | 2.43 | 0.48 |
| 55:QY:186:ARG:HB3 | 55:QY:312:PHE:HD2 | 1.79 | 0.48 |
| 1:RA:1005:C:H2' | 1:RA:1006:C:C6 | 2.49 | 0.48 |
| 1:RA:848:G:H2' | 1:RA:849:A:C8 | 2.48 | 0.48 |
| 12:RQ:109:VAL:HG13 | 12:RQ:113:GLN:HB2 | 1.96 | 0.48 |
| 33:XB:218:ALA:O | 33:XB:222:ILE:HG23 | 2.13 | 0.48 |
| 25:Y3:29:ARG:HB2 | 25:Y3:30:ARG:HD3 | 1.95 | 0.48 |
| 1:YA:1165:U:H2' | 1:YA:1166:C:C6 | 2.48 | 0.48 |
| 11:YP:97:PRO:HD3 | 11:YP:126:VAL:O | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:QB:231:GLU:HB3 | 33:QB:232:PRO:HD3 | 1.96 | 0.48 |
| 35:QD:166:LYS:HB2 | 35:QD:168:ARG:NH2 | 2.28 | 0.48 |
| 1:RA:1104:C:H2' | 1:RA:1105:U:C6 | 2.48 | 0.48 |
| 1:RA:218:A:C2 | 1:RA:235:U:H4' | 2.48 | 0.48 |
| 32:XA:1158:C:O2 | 32:XA:1158:C:H2' | 2.12 | 0.48 |
| 40:XI:31:GLN:HG3 | 40:XI:36:TYR:HB2 | 1.95 | 0.48 |
| 1:YA:569:U:C4 | 1:YA:570:G:C6 | 3.02 | 0.48 |
| 1:YA:587:C:OP2 | 11:YP:21:ARG:NH2 | 2.46 | 0.48 |
| 4:YE:18:ASP:HB3 | 15:YT:82:LEU:HD21 | 1.95 | 0.48 |
| 5:YF:130:ALA:HB3 | 5:YF:142:TRP:HD1 | 1.79 | 0.48 |
| 9:YN:4:TYR:CD2 | 16:YU:100:VAL:HG11 | 2.48 | 0.48 |
| 32:QA:1002:G:C6 | 32:QA:1003:G:C2 | 3.02 | 0.48 |
| 32:QA:337:C:H2' | 32:QA:338:A:C8 | 2.48 | 0.48 |
| 1:RA:1739:U:HO2' | 1:RA:1740:G:H8 | 1.59 | 0.48 |
| 1:RA:721:C:H2' | 1:RA:722:A:C8 | 2.49 | 0.48 |
| 8:RI:81:VAL:O | 8:RI:146:ALA:HA | 2.14 | 0.48 |
| 32:XA:511:C:HO2' | 32:XA:512:U:H6 | 1.59 | 0.48 |
| 34:XC:9:GLY:HA3 | 45:XN:49:HIS:HA | 1.95 | 0.48 |
| 1:YA:2079:U:OP1 | 23:Y1:21:ARG:NH2 | 2.47 | 0.48 |
| 1:YA:2755:C:C2 | 31:Y9:19:ARG:HD3 | 2.49 | 0.48 |
| 32:QA:457:C:H2' | 32:QA:458:C:C6 | 2.49 | 0.48 |
| 47:QP:20:VAL:HG21 | 47:QP:32:TYR:CG | 2.49 | 0.48 |
| 55:QY:219:PRO:O | 55:QY:221:ASP:N | 2.46 | 0.48 |
| 1:RA:2010:G:H5'' | 18:RW:42:ARG:HB2 | 1.96 | 0.48 |
| 1:RA:2849:U:O4 | 15:RT:23:ARG:NH2 | 2.46 | 0.48 |
| 1:RA:637:A:OP1 | 11:RP:133:SER:OG | 2.23 | 0.48 |
| 1:RA:873:G:H1 | 1:RA:904:C:H42 | 1.60 | 0.48 |
| 12:RQ:21:THR:CG2 | 12:RQ:101:ARG:HB2 | 2.43 | 0.48 |
| 32:XA:1036:G:H3' | 32:XA:1037:C:C6 | 2.49 | 0.48 |
| 41:XJ:78:ASN:O | 41:XJ:80:LYS:N | 2.46 | 0.48 |
| 1:YA:1570:A:H2' | 1:YA:1571:A:C8 | 2.49 | 0.48 |
| 1:YA:273(A):G:N7 | 1:YA:421:U:H2' | 2.29 | 0.48 |
| 1:YA:1826:G:H4' | 3:YD:242:ARG:CZ | 2.44 | 0.48 |
| 5:YF:140:LEU:HD21 | 5:YF:170:LEU:HD11 | 1.95 | 0.48 |
| 8:YI:110:ASP:N | 8:YI:130:TYR:OH | 2.37 | 0.48 |
| 32:QA:974:A:OP1 | 32:QA:974:A:H8 | 1.96 | 0.48 |
| 38:QG:26:PHE:O | 38:QG:30:ILE:HG13 | 2.14 | 0.48 |
| 26:R4:68:ARG:HA | 26:R4:68:ARG:NH2 | 2.29 | 0.48 |
| 1:RA:2286:A:H4' | 1:RA:2287:A:O4' | 2.14 | 0.48 |
| 1:RA:2478:A:H5' | 31:R9:31:LYS:HE2 | 1.96 | 0.48 |
| 32:XA:109:A:C6 | 32:XA:326:G:C6 | 3.02 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:Y4:20:ASN:ND2 | 26:Y4:38:LYS:HG3 | 2.28 | 0.48 |
| 1:YA:2115:G:N2 | 1:YA:2171:A:H61 | 2.12 | 0.48 |
| 1:YA:2507:C:O4' | 55:XY:238:ASN:HB3 | 2.13 | 0.48 |
| 1:YA:1803:A:O2' | 3:YD:259:THR:HG21 | 2.13 | 0.48 |
| 6:YG:35:GLU:HG3 | 6:YG:36:LYS:HE3 | 1.95 | 0.48 |
| 21:YZ:179:ASP:O | 21:YZ:182:LYS:HG2 | 2.14 | 0.48 |
| 34:QC:50:ALA:HB1 | 34:QC:70:VAL:HG21 | 1.96 | 0.48 |
| 47:QP:75:ARG:HG3 | 47:QP:80:PHE:HD2 | 1.78 | 0.48 |
| 51:QT:18:GLN:O | 51:QT:22:ARG:HG3 | 2.13 | 0.48 |
| 1:RA:2611:U:C4 | 27:R5:3:LYS:HG2 | 2.48 | 0.48 |
| 1:RA:1410:G:H2' | 1:RA:1411:C:C6 | 2.48 | 0.48 |
| 5:RF:165:ARG:HA | 5:RF:168:ARG:CD | 2.44 | 0.48 |
| 5:RF:167:ALA:HB1 | 5:RF:173:VAL:HG11 | 1.96 | 0.48 |
| 32:XA:396:G:O2' | 32:XA:398:C:OP1 | 2.21 | 0.48 |
| 32:XA:972:C:H4' | 41:XJ:57:LYS:HB2 | 1.96 | 0.48 |
| 33:XB:222:ILE:HG13 | 33:XB:223:ILE:N | 2.29 | 0.48 |
| 55:XY:177:PHE:O | 55:XY:321:ARG:NH1 | 2.47 | 0.48 |
| 12:YQ:77:LYS:NZ | 12:YQ:86:GLY:O | 2.47 | 0.48 |
| 32:QA:1516:G:N1 | 32:QA:1519:MA6:OP2 | 2.46 | 0.47 |
| 33:QB:21:ARG:H | 33:QB:21:ARG:HD3 | 1.78 | 0.47 |
| 32:QA:1316:G:H5'' | 45:QN:17:LYS:NZ | 2.29 | 0.47 |
| 1:RA:1814:G:H4' | 3:RD:51:VAL:HG21 | 1.95 | 0.47 |
| 1:RA:2262:U:H4' | 1:RA:2328:A:C2 | 2.49 | 0.47 |
| 18:RW:46:PHE:O | 18:RW:50:VAL:HG23 | 2.14 | 0.47 |
| 33:XB:9:GLU:O | 33:XB:11:LEU:N | 2.47 | 0.47 |
| 28:Y6:35:GLU:OE2 | 28:Y6:50:ARG:NH1 | 2.46 | 0.47 |
| 1:YA:2152:G:H2' | 1:YA:2153:G:H8 | 1.78 | 0.47 |
| 17:YV:52:VAL:CG2 | 17:YV:55:ALA:HB3 | 2.44 | 0.47 |
| 21:YZ:126:VAL:HG11 | 21:YZ:161:VAL:HG13 | 1.96 | 0.47 |
| 32:QA:384:G:H2' | 32:QA:385:C:C6 | 2.48 | 0.47 |
| 35:QD:178:VAL:HG12 | 35:QD:179:GLU:H | 1.79 | 0.47 |
| 40:QI:16:ARG:H | 40:QI:64:THR:HG22 | 1.78 | 0.47 |
| 44:QM:11:ARG:HA | 44:QM:45:VAL:HB | 1.96 | 0.47 |
| 55:QY:114:GLU:OE2 | 55:QY:294:ARG:HD3 | 2.13 | 0.47 |
| 1:RA:1070:A:H2' | 1:RA:1071:G:C8 | 2.48 | 0.47 |
| 1:RA:2137:C:C2 | 1:RA:2154:G:N1 | 2.82 | 0.47 |
| 1:RA:2683:C:OP1 | 15:RT:53:ARG:NH2 | 2.47 | 0.47 |
| 1:RA:57:C:H2' | 1:RA:58:G:O4' | 2.14 | 0.47 |
| 3:RD:72:LYS:HG3 | 3:RD:103:ARG:NH2 | 2.29 | 0.47 |
| 5:RF:178:PRO:HB2 | 5:RF:201:VAL:HG21 | 1.95 | 0.47 |
| 10:RO:73:ASP:HB2 | 15:RT:82:LEU:HD13 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 32:XA:972:C:O5' | 41:XJ:57:LYS:HG2 | 2.14 | 0.47 |
| 33:XB:28:PHE:O | 33:XB:32:ILE:HG13 | 2.14 | 0.47 |
| 34:XC:8:ILE:HG23 | 34:XC:16:ARG:HG2 | 1.95 | 0.47 |
| 39:XH:86:ILE:HG12 | 39:XH:135:CYS:HA | 1.96 | 0.47 |
| 40:XI:21:PRO:HA | 40:XI:59:PHE:HA | 1.96 | 0.47 |
| 26:Y4:24:THR:OG1 | 26:Y4:25:TYR:N | 2.47 | 0.47 |
| 1:YA:2420:C:OP1 | 30:Y8:34:TRP:HB3 | 2.14 | 0.47 |
| 1:YA:1278:A:OP1 | 13:YR:36:THR:HG23 | 2.14 | 0.47 |
| 1:YA:2086:U:H2' | 1:YA:2087:G:C8 | 2.49 | 0.47 |
| 32:QA:1402:4OC:H6 | 32:QA:1402:4OC:O5' | 2.13 | 0.47 |
| 28:R6:34:LEU:HB2 | 28:R6:51:GLU:HB2 | 1.95 | 0.47 |
| 11:RP:50:ARG:HD3 | 30:R8:7:HIS:CD2 | 2.50 | 0.47 |
| 1:RA:1300:U:H4' | 1:RA:1301:A:H5' | 1.95 | 0.47 |
| 1:RA:2098:U:H2' | 1:RA:2099:U:O4' | 2.14 | 0.47 |
| 1:RA:2567:G:H2' | 1:RA:2568:C:C6 | 2.49 | 0.47 |
| 1:RA:2889:C:H3' | 1:RA:2891:G:C8 | 2.49 | 0.47 |
| 20:RY:76:CYS:SG | 20:RY:78:ALA:HB3 | 2.54 | 0.47 |
| 21:RZ:103:ARG:HD2 | 21:RZ:136:PHE:CD2 | 2.49 | 0.47 |
| 32:XA:1518:MA6:H93 | 32:XA:1519:MA6:H102 | 1.96 | 0.47 |
| 40:XI:100:GLY:O | 40:XI:103:THR:HG22 | 2.14 | 0.47 |
| 1:YA:1405:U:H2' | 1:YA:1406:U:C6 | 2.49 | 0.47 |
| 1:YA:2342:C:O2' | 1:YA:2374:C:H5'' | 2.13 | 0.47 |
| 1:YA:2401:U:H3' | 1:YA:2402:C:C6 | 2.48 | 0.47 |
| 1:YA:1805:U:O2 | 3:YD:50:THR:HB | 2.15 | 0.47 |
| 7:YH:20:ALA:HB1 | 7:YH:21:PRO:HD2 | 1.96 | 0.47 |
| 32:QA:266:G:H2' | 32:QA:266:G:N3 | 2.29 | 0.47 |
| 33:QB:95:GLN:HB3 | 33:QB:96:ARG:H | 1.58 | 0.47 |
| 32:QA:1316:G:O2' | 45:QN:18:VAL:HG11 | 2.14 | 0.47 |
| 44:QM:86:CYS:HB2 | 50:QS:73:GLU:HB3 | 1.96 | 0.47 |
| 1:RA:579:G:H2' | 1:RA:580:C:C6 | 2.49 | 0.47 |
| 9:RN:15:LEU:HD12 | 9:RN:137:LYS:HG2 | 1.96 | 0.47 |
| 32:XA:1333:A:H2' | 32:XA:1334:G:O4' | 2.13 | 0.47 |
| 33:XB:71:VAL:HG23 | 33:XB:164:VAL:HA | 1.96 | 0.47 |
| 38:XG:65:ALA:HB1 | 38:XG:127:ALA:HB3 | 1.96 | 0.47 |
| 38:XG:26:PHE:O | 38:XG:30:ILE:HG13 | 2.15 | 0.47 |
| 50:XS:77:THR:HG23 | 50:XS:78:ARG:HG3 | 1.97 | 0.47 |
| 1:YA:1171:G:N2 | 1:YA:1178:C:O2 | 2.47 | 0.47 |
| 1:YA:2359:C:H2' | 1:YA:2360:A:O4' | 2.13 | 0.47 |
| 5:YF:10:PRO:HB3 | 5:YF:17:ARG:HE | 1.80 | 0.47 |
| 1:YA:1665:A:H4' | 10:YO:67:LYS:HB2 | 1.96 | 0.47 |
| 1:RA:11:G:C2' | 1:RA:12:U:H5' | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:RA:2391:G:O6 | 1:RA:2425:A:H8 | 1.97 | 0.47 |
| 1:RA:918:A:H5'' | 2:RB:98:G:O2' | 2.14 | 0.47 |
| 3:RD:2:ALA:N | 3:RD:200:ASP:OD2 | 2.47 | 0.47 |
| 32:XA:1040:U:H2' | 32:XA:1041:A:H5'' | 1.96 | 0.47 |
| 55:XY:341:ILE:HA | 55:XY:344:ILE:HD12 | 1.96 | 0.47 |
| 1:YA:2031:A:C6 | 1:YA:2498:C:H1' | 2.49 | 0.47 |
| 6:YG:55:LYS:HD3 | 6:YG:150:ASP:OD2 | 2.14 | 0.47 |
| 21:YZ:10:ARG:HH21 | 21:YZ:26:GLY:H | 1.61 | 0.47 |
| 21:YZ:150:LEU:HB3 | 21:YZ:171:ILE:HD11 | 1.96 | 0.47 |
| 32:QA:630:G:O2' | 32:QA:631:G:H5' | 2.14 | 0.47 |
| 33:QB:115:LEU:HD12 | 33:QB:142:LEU:HD12 | 1.95 | 0.47 |
| 33:QB:16:HIS:CG | 33:QB:17:PHE:N | 2.82 | 0.47 |
| 35:QD:166:LYS:H | 35:QD:168:ARG:HH21 | 1.62 | 0.47 |
| 48:QQ:78:GLU:HG2 | 48:QQ:79:SER:N | 2.28 | 0.47 |
| 1:RA:1058:G:H1 | 1:RA:1080:C:H42 | 1.62 | 0.47 |
| 1:RA:523:C:H4' | 1:RA:540:C:O2 | 2.14 | 0.47 |
| 1:RA:574:C:N3 | 4:RE:145:LYS:NZ | 2.42 | 0.47 |
| 1:RA:2820:A:OP2 | 13:RR:2:ARG:NH2 | 2.47 | 0.47 |
| 32:XA:1032:G:C2' | 32:XA:1033:G:H5' | 2.44 | 0.47 |
| 32:XA:1286:A:H2' | 32:XA:1287:A:H4' | 1.97 | 0.47 |
| 38:XG:111:ARG:HD3 | 38:XG:113:GLU:OE2 | 2.15 | 0.47 |
| 4:YE:98:PRO:HD3 | 4:YE:175:VAL:HG12 | 1.97 | 0.47 |
| 14:YS:27:SER:HA | 14:YS:88:ASP:HB3 | 1.96 | 0.47 |
| 32:QA:1003:G:C2 | 32:QA:1004:A:H1' | 2.50 | 0.47 |
| 36:QE:90:VAL:O | 36:QE:120:THR:HA | 2.14 | 0.47 |
| 26:R4:50:VAL:HG21 | 44:QM:64:TRP:C | 2.35 | 0.47 |
| 1:RA:1899:G:N3 | 1:RA:1899:G:H2' | 2.30 | 0.47 |
| 1:RA:2111:C:H42 | 1:RA:2147:G:H22 | 1.62 | 0.47 |
| 1:RA:2122:U:H2' | 1:RA:2123:G:C8 | 2.50 | 0.47 |
| 1:RA:752:A:H3' | 29:R7:1:MET:HE2 | 1.95 | 0.47 |
| 11:RP:94:GLU:HG3 | 11:RP:124:LYS:HD3 | 1.97 | 0.47 |
| 19:RX:44:GLU:HG3 | 19:RX:51:VAL:HG23 | 1.97 | 0.47 |
| 32:XA:1036:G:H3' | 32:XA:1037:C:H6 | 1.79 | 0.47 |
| 32:XA:1118:C:P | 40:XI:104:ARG:HH11 | 2.37 | 0.47 |
| 32:XA:542:G:OP1 | 35:XD:10:ARG:NH1 | 2.43 | 0.47 |
| 35:XD:199:ASN:OD1 | 35:XD:201:GLN:HB2 | 2.14 | 0.47 |
| 50:XS:27:GLU:OE1 | 50:XS:47:HIS:NE2 | 2.46 | 0.47 |
| 1:YA:1092:C:H6 | 1:YA:1092:C:OP2 | 1.98 | 0.47 |
| 3:YD:16:MET:HG3 | 3:YD:206:LEU:O | 2.15 | 0.47 |
| 15:YT:118:ARG:HG2 | 32:XA:1442(B):G:C8 | 2.49 | 0.47 |
| 32:QA:1027:C:H2' | 32:QA:1028:C:C5 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:QC:8:ILE:HD12 | 34:QC:16:ARG:HD3 | 1.97 | 0.47 |
| 1:RA:1359:A:H61 | 1:RA:1372:U:H3 | 1.63 | 0.47 |
| 7:RH:7:LEU:O | 7:RH:69:ARG:NH1 | 2.46 | 0.47 |
| 8:RI:72:LEU:HD13 | 8:RI:140:LEU:HD23 | 1.95 | 0.47 |
| 32:XA:961:U:OP2 | 32:XA:1223:C:O2' | 2.26 | 0.47 |
| 34:XC:140:ARG:HB2 | 34:XC:140:ARG:NH1 | 2.30 | 0.47 |
| 41:XJ:38:ILE:HG12 | 41:XJ:71:LEU:HB3 | 1.96 | 0.47 |
| 32:XA:950:U:OP2 | 44:XM:102:ARG:HD3 | 2.15 | 0.47 |
| 1:YA:2336:A:H61 | 22:Y0:43:THR:HG22 | 1.79 | 0.47 |
| 1:YA:2158:A:H1' | 1:YA:2159:G:C8 | 2.50 | 0.47 |
| 3:YD:12:SER:HB3 | 3:YD:208:LYS:HB3 | 1.97 | 0.47 |
| 7:YH:12:PRO:O | 7:YH:15:VAL:HG22 | 2.15 | 0.47 |
| 8:YI:50:ARG:HB3 | 8:YI:50:ARG:HE | 1.40 | 0.47 |
| 17:YV:15:GLU:O | 17:YV:18:LEU:HB2 | 2.15 | 0.47 |
| 20:YY:13:VAL:HB | 20:YY:72:VAL:HG13 | 1.95 | 0.47 |
| 32:QA:1218:C:H2' | 32:QA:1219:U:C6 | 2.50 | 0.47 |
| 32:QA:1279:A:O2' | 32:QA:1282:C:N4 | 2.48 | 0.47 |
| 32:QA:186:C:H2' | 32:QA:187:C:H6 | 1.80 | 0.47 |
| 39:QH:95:VAL:HB | 39:QH:99:GLU:HB2 | 1.97 | 0.47 |
| 43:QL:33:ARG:HD2 | 43:QL:33:ARG:HA | 1.62 | 0.47 |
| 1:RA:1817:G:OP1 | 3:RD:88:ARG:NH2 | 2.33 | 0.47 |
| 12:RQ:18:LYS:O | 12:RQ:98:LYS:NZ | 2.33 | 0.47 |
| 32:XA:130:A:O2' | 32:XA:131:C:O5' | 2.31 | 0.47 |
| 55:XY:133:ARG:O | 55:XY:137:ARG:HG2 | 2.14 | 0.47 |
| 1:YA:1125:G:C6 | 1:YA:1126:A:N6 | 2.83 | 0.47 |
| 1:YA:272(O):C:H2' | 1:YA:272(P):C:C6 | 2.49 | 0.47 |
| 1:YA:2823:A:OP1 | 4:YE:113:PHE:HB2 | 2.13 | 0.47 |
| 32:QA:179:A:H2' | 32:QA:180:U:C6 | 2.50 | 0.47 |
| 32:QA:745:C:H2' | 32:QA:746:A:C8 | 2.49 | 0.47 |
| 44:QM:40:ASN:HB3 | 44:QM:43:THR:HG23 | 1.96 | 0.47 |
| 46:QO:26:GLU:OE1 | 46:QO:77:ARG:NE | 2.48 | 0.47 |
| 1:RA:2104:G:O6 | 1:RA:2186:G:C4 | 2.67 | 0.47 |
| 1:RA:228:A:H8 | 1:RA:229:A:H5' | 1.79 | 0.47 |
| 1:RA:1805:U:O2 | 3:RD:50:THR:HB | 2.14 | 0.47 |
| 14:RS:27:SER:HA | 14:RS:88:ASP:HB3 | 1.96 | 0.47 |
| 55:XY:138:TYR:HD1 | 55:XY:337:LEU:H | 1.63 | 0.47 |
| 1:YA:1608:A:H1' | 1:YA:1610:A:OP2 | 2.15 | 0.47 |
| 1:YA:2122:U:H3 | 1:YA:2176:A:N6 | 2.13 | 0.47 |
| 1:YA:2552:2MU:H6 | 1:YA:2552:2MU:O5' | 2.15 | 0.47 |
| 1:YA:2836:U:H2' | 1:YA:2837:G:C8 | 2.49 | 0.47 |
| 1:YA:295:G:OP1 | 20:YY:1:MET:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:YA:529:A:OP2 | 9:YN:114:ARG:NH2 | 2.47 | 0.47 |
| 1:YA:581:C:H2' | 1:YA:582:G:C8 | 2.49 | 0.47 |
| 1:YA:57:C:H2' | 1:YA:58:G:O4' | 2.14 | 0.47 |
| 1:YA:2811:G:OP1 | 4:YE:60:ASN:HB2 | 2.14 | 0.47 |
| 5:YF:29:ASN:HB3 | 5:YF:112:MET:HE1 | 1.97 | 0.47 |
| 6:YG:83:ARG:O | 6:YG:86:MET:HB2 | 2.15 | 0.47 |
| 8:YI:72:LEU:O | 8:YI:75:LEU:HD22 | 2.15 | 0.47 |
| 40:QI:33:PHE:CE1 | 40:QI:43:ALA:HB1 | 2.50 | 0.47 |
| 53:QV:43:A:H2' | 53:QV:44:A:C8 | 2.49 | 0.47 |
| 53:QV:21:A:H61 | 53:QV:46:G:H2' | 1.80 | 0.47 |
| 1:RA:1053:C:H4' | 1:RA:1054:A:OP1 | 2.15 | 0.47 |
| 1:RA:1139:G:O2' | 1:RA:1143:A:N1 | 2.37 | 0.47 |
| 1:RA:1657:C:H2' | 1:RA:1658:C:C6 | 2.50 | 0.47 |
| 1:RA:1936:A:OP2 | 1:RA:1962:5MC:N4 | 2.37 | 0.47 |
| 1:RA:1939:5MU:OP1 | 1:RA:2604:U:O2' | 2.33 | 0.47 |
| 1:RA:2528:U:H2' | 1:RA:2530:A:O5' | 2.15 | 0.47 |
| 1:RA:668:G:H5' | 1:RA:669:G:OP2 | 2.14 | 0.47 |
| 18:RW:4:LYS:HB2 | 18:RW:106:ILE:HG12 | 1.97 | 0.47 |
| 20:RY:6:HIS:HE1 | 20:RY:72:VAL:O | 1.98 | 0.47 |
| 21:RZ:125:LEU:HB3 | 21:RZ:165:VAL:HG13 | 1.96 | 0.47 |
| 32:XA:1142:G:H2' | 32:XA:1143:G:O4' | 2.14 | 0.47 |
| 32:XA:1342:C:H2' | 32:XA:1343:G:H8 | 1.80 | 0.47 |
| 32:XA:662:G:H2' | 32:XA:663:A:H8 | 1.80 | 0.47 |
| 32:XA:828:A:H2' | 32:XA:829:G:O4' | 2.15 | 0.47 |
| 40:XI:51:ARG:HG2 | 40:XI:56:LEU:HD21 | 1.97 | 0.47 |
| 51:XT:56:MET:HE2 | 51:XT:84:LEU:HD22 | 1.97 | 0.47 |
| 1:YA:1914:C:OP1 | 55:XY:116:ARG:NH2 | 2.48 | 0.47 |
| 1:YA:1028:A:N7 | 1:YA:1126:A:N7 | 2.63 | 0.47 |
| 1:YA:1252:G:C2 | 1:YA:1253:A:C2 | 3.03 | 0.47 |
| 1:YA:1514:U:H2' | 1:YA:1515:G:H8 | 1.79 | 0.47 |
| 1:YA:1683:C:H2' | 1:YA:1684:C:C6 | 2.50 | 0.47 |
| 1:YA:2111:C:H42 | 1:YA:2147:G:H22 | 1.62 | 0.47 |
| 1:YA:859:G:O2' | 1:YA:916:G:O6 | 2.31 | 0.47 |
| 1:YA:1814:G:H4' | 3:YD:51:VAL:HG21 | 1.97 | 0.47 |
| 4:YE:14:ILE:HG13 | 4:YE:21:VAL:HG13 | 1.96 | 0.47 |
| 20:YY:37:VAL:HG21 | 20:YY:72:VAL:HG21 | 1.96 | 0.47 |
| 32:QA:1074:G:O2' | 32:QA:1101:A:N1 | 2.37 | 0.46 |
| 43:QL:71:PRO:O | 43:QL:102:ARG:NH1 | 2.47 | 0.46 |
| 53:QV:50:U:H3 | 53:QV:64:G:H1 | 1.62 | 0.46 |
| 1:RA:2478:A:H5' | 31:R9:31:LYS:HG2 | 1.98 | 0.46 |
| 1:RA:2438:U:O2' | 1:RA:2440:C:OP1 | 2.21 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:RA:2849:U:H4' | 1:RA:2868:A:C2 | 2.50 | 0.46 |
| 1:RA:375:C:H2' | 1:RA:376:C:C6 | 2.50 | 0.46 |
| 32:XA:41:G:H2' | 32:XA:42:G:C8 | 2.50 | 0.46 |
| 32:XA:8:A:N6 | 35:XD:205:GLU:O | 2.46 | 0.46 |
| 41:XJ:11:PHE:CE1 | 41:XJ:67:THR:HG22 | 2.48 | 0.46 |
| 1:YA:2611:U:C4 | 27:Y5:3:LYS:HG2 | 2.50 | 0.46 |
| 1:YA:746:A:H2' | 1:YA:2612:C:H5'' | 1.97 | 0.46 |
| 1:YA:98:G:H5' | 24:Y2:3:LEU:HG | 1.97 | 0.46 |
| 6:YG:36:LYS:HE2 | 6:YG:95:ARG:HH12 | 1.81 | 0.46 |
| 8:YI:4:ILE:HD11 | 8:YI:44:LEU:HD13 | 1.96 | 0.46 |
| 11:YP:97:PRO:HA | 11:YP:112:LEU:HD12 | 1.96 | 0.46 |
| 11:YP:91:PHE:CE2 | 11:YP:99:LEU:HD21 | 2.50 | 0.46 |
| 1:YA:954:G:H5'' | 12:YQ:13:GLN:HB3 | 1.96 | 0.46 |
| 32:QA:1124:G:N2 | 32:QA:1125:U:O4 | 2.47 | 0.46 |
| 32:QA:335:C:H2' | 32:QA:336:C:C6 | 2.50 | 0.46 |
| 55:QY:133:ARG:O | 55:QY:137:ARG:HG2 | 2.15 | 0.46 |
| 1:RA:2850:A:N7 | 1:RA:2868:A:O2' | 2.37 | 0.46 |
| 1:RA:824:A:H1' | 1:RA:2358:G:N7 | 2.31 | 0.46 |
| 37:XF:35:ALA:HA | 37:XF:67:MET:HB3 | 1.97 | 0.46 |
| 49:XR:33:ASP:OD2 | 49:XR:36:ASN:HB2 | 2.15 | 0.46 |
| 1:YA:1657:C:H2' | 1:YA:1658:C:C6 | 2.50 | 0.46 |
| 1:YA:1756:G:H4' | 1:YA:1758:G:O4' | 2.15 | 0.46 |
| 1:YA:2306:C:C4 | 1:YA:2307:G:C6 | 3.04 | 0.46 |
| 5:YF:132:VAL:CG2 | 5:YF:163:VAL:HG22 | 2.44 | 0.46 |
| 32:QA:18:C:H4' | 32:QA:1078:U:O2 | 2.15 | 0.46 |
| 32:QA:1395:C:O2' | 32:QA:1401:G:O2' | 2.15 | 0.46 |
| 32:QA:1118:C:P | 40:QI:104:ARG:HH11 | 2.39 | 0.46 |
| 47:QP:43:LYS:HG2 | 47:QP:48:TRP:CE2 | 2.50 | 0.46 |
| 55:QY:221:ASP:HB3 | 55:QY:250:PRO:HD3 | 1.96 | 0.46 |
| 1:RA:2149:G:C2 | 1:RA:2150:U:H1' | 2.50 | 0.46 |
| 1:RA:272(O):C:H2' | 1:RA:272(P):C:C6 | 2.50 | 0.46 |
| 3:RD:17:THR:O | 3:RD:211:ARG:NH2 | 2.38 | 0.46 |
| 8:RI:72:LEU:C | 8:RI:74:ASN:H | 2.18 | 0.46 |
| 32:XA:60:A:H4' | 32:XA:61:G:O5' | 2.16 | 0.46 |
| 32:XA:784:C:H2' | 32:XA:785:G:O4' | 2.16 | 0.46 |
| 33:XB:19:HIS:CG | 33:XB:20:GLU:N | 2.83 | 0.46 |
| 42:XK:27:ASN:OD1 | 42:XK:28:THR:N | 2.46 | 0.46 |
| 55:XY:233:GLY:HA3 | 55:XY:237:VAL:HG23 | 1.97 | 0.46 |
| 1:YA:1514:U:H2' | 1:YA:1515:G:C8 | 2.51 | 0.46 |
| 1:YA:1557:C:H5'' | 1:YA:1558:A:OP2 | 2.15 | 0.46 |
| 1:YA:184:C:H2' | 1:YA:185:U:C6 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:YD:108:PRO:HB3 | 3:YD:143:HIS:HE1 | 1.78 | 0.46 |
| 7:YH:41:MET:N | 7:YH:41:MET:SD | 2.88 | 0.46 |
| 32:QA:840:C:H4' | 32:QA:841:U:OP1 | 2.16 | 0.46 |
| 40:QI:17:VAL:HG23 | 40:QI:63:ILE:HG12 | 1.96 | 0.46 |
| 1:RA:1239:G:H2' | 1:RA:1240:U:O4' | 2.15 | 0.46 |
| 1:RA:1385:G:O2' | 1:RA:1396:U:O2 | 2.31 | 0.46 |
| 1:RA:1404:C:H2' | 1:RA:1405:U:H6 | 1.80 | 0.46 |
| 1:RA:1514:U:H2' | 1:RA:1515:G:H8 | 1.81 | 0.46 |
| 1:RA:1686:C:H2' | 1:RA:1687:G:O4' | 2.15 | 0.46 |
| 1:RA:2158:A:H1' | 1:RA:2159:G:C8 | 2.50 | 0.46 |
| 1:RA:2180:U:H2' | 1:RA:2181:G:C8 | 2.50 | 0.46 |
| 1:RA:1971:A:C4 | 3:RD:241:PRO:HD3 | 2.50 | 0.46 |
| 6:RG:43:LEU:HD23 | 6:RG:53:LEU:HD12 | 1.98 | 0.46 |
| 8:RI:117:GLU:HG3 | 8:RI:118:LYS:N | 2.31 | 0.46 |
| 9:RN:20:GLY:HA2 | 9:RN:61:ARG:HD3 | 1.97 | 0.46 |
| 32:XA:1305:G:H22 | 32:XA:1331:G:H1' | 1.79 | 0.46 |
| 40:XI:8:GLY:HA2 | 40:XI:79:LEU:HD23 | 1.96 | 0.46 |
| 55:XY:114:GLU:OE2 | 55:XY:294:ARG:HD3 | 2.15 | 0.46 |
| 23:Y1:51:VAL:HG12 | 23:Y1:53:VAL:HG23 | 1.97 | 0.46 |
| 1:YA:1163:G:OP1 | 17:YV:24:LYS:NZ | 2.31 | 0.46 |
| 1:YA:2134:A:C5 | 1:YA:2157:G:H5' | 2.50 | 0.46 |
| 1:YA:286:C:H2' | 1:YA:287:C:C6 | 2.49 | 0.46 |
| 4:YE:170:LEU:HD23 | 4:YE:184:VAL:HG11 | 1.96 | 0.46 |
| 15:YT:118:ARG:HG2 | 32:XA:1442(B):G:N9 | 2.30 | 0.46 |
| 15:YT:39:ARG:NH2 | 32:XA:345:C:OP2 | 2.46 | 0.46 |
| 21:YZ:125:LEU:HG | 21:YZ:164:ALA:HB3 | 1.96 | 0.46 |
| 32:QA:551:U:H2' | 32:QA:552:U:C6 | 2.50 | 0.46 |
| 32:QA:664:G:N2 | 32:QA:741:G:H1 | 2.06 | 0.46 |
| 32:QA:765:G:N1 | 32:QA:812:C:O2' | 2.44 | 0.46 |
| 32:QA:881:G:OP2 | 43:QL:12:ARG:NH2 | 2.49 | 0.46 |
| 33:QB:69:LEU:HB3 | 33:QB:162:ILE:HG22 | 1.97 | 0.46 |
| 33:QB:91:PRO:HG2 | 33:QB:155:LEU:HD23 | 1.96 | 0.46 |
| 39:QH:36:LEU:HD12 | 39:QH:59:LEU:HD13 | 1.97 | 0.46 |
| 27:R5:35:GLU:HG3 | 27:R5:51:TYR:CB | 2.45 | 0.46 |
| 1:RA:249:C:O2 | 30:R8:12:LYS:NZ | 2.41 | 0.46 |
| 1:RA:300:A:H1' | 1:RA:319:C:H1' | 1.98 | 0.46 |
| 1:RA:839:U:H2' | 1:RA:840:C:C6 | 2.49 | 0.46 |
| 1:RA:1278:A:OP1 | 13:RR:36:THR:HG23 | 2.15 | 0.46 |
| 55:XY:329:LEU:HG | 55:XY:330:ASP:N | 2.30 | 0.46 |
| 1:YA:1041:C:N4 | 1:YA:1114:G:H1 | 2.00 | 0.46 |
| 1:YA:1525:G:H2' | 1:YA:1526:G:H8 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:2315:G:H2' | 1:YA:2316:C:C6 | 2.51 | 0.46 |
| 1:YA:7:G:H2' | 1:YA:8:A:C8 | 2.50 | 0.46 |
| 2:YB:42:C:O2 | 6:YG:93:THR:N | 2.40 | 0.46 |
| 6:YG:106:LEU:HA | 6:YG:110:ALA:HB3 | 1.96 | 0.46 |
| 9:YN:120:LEU:HD11 | 9:YN:122:VAL:HG23 | 1.98 | 0.46 |
| 9:YN:137:LYS:HD3 | 9:YN:138:LEU:N | 2.30 | 0.46 |
| 32:QA:1036:G:H5' | 32:QA:1037:C:OP2 | 2.16 | 0.46 |
| 32:QA:540:G:H2' | 32:QA:541:G:O4' | 2.16 | 0.46 |
| 32:QA:564:C:O2' | 39:QH:91:ARG:NH2 | 2.45 | 0.46 |
| 32:QA:757:U:H2' | 32:QA:758:G:O4' | 2.16 | 0.46 |
| 33:QB:146:GLN:O | 33:QB:150:SER:HB3 | 2.15 | 0.46 |
| 32:QA:4:U:O4 | 39:QH:105:ARG:HA | 2.16 | 0.46 |
| 32:QA:1302:U:H5 | 44:QM:17:VAL:HG21 | 1.80 | 0.46 |
| 48:QQ:10:VAL:HG13 | 48:QQ:19:VAL:HB | 1.98 | 0.46 |
| 1:RA:1062:G:O2' | 1:RA:1063:G:H5' | 2.16 | 0.46 |
| 2:RB:41:U:H5 | 6:RG:70:VAL:O | 1.98 | 0.46 |
| 6:RG:7:LEU:HD13 | 6:RG:100:TRP:CE3 | 2.50 | 0.46 |
| 18:RW:14:PRO:HG2 | 18:RW:78:GLU:CG | 2.42 | 0.46 |
| 32:XA:555:C:H2' | 32:XA:556:C:C6 | 2.51 | 0.46 |
| 35:XD:61:LYS:HD2 | 35:XD:207:TYR:OH | 2.15 | 0.46 |
| 50:XS:50:ALA:HA | 50:XS:58:VAL:O | 2.16 | 0.46 |
| 55:XY:109:ARG:CZ | 55:XY:209:LEU:HD13 | 2.46 | 0.46 |
| 55:XY:326:LEU:HD13 | 55:XY:328:ARG:HB2 | 1.98 | 0.46 |
| 1:YA:2285:C:OP2 | 28:Y6:26:ASN:ND2 | 2.42 | 0.46 |
| 1:YA:579:G:H2' | 1:YA:580:C:C6 | 2.50 | 0.46 |
| 1:YA:886:C:O2' | 1:YA:889:C:N4 | 2.46 | 0.46 |
| 33:QB:76:GLN:HE21 | 33:QB:206:ASP:HA | 1.81 | 0.46 |
| 44:QM:54:VAL:HA | 44:QM:57:ARG:HB3 | 1.98 | 0.46 |
| 53:QV:19:G:H5' | 53:QV:20:U:H5 | 1.81 | 0.46 |
| 22:R0:23:VAL:HG22 | 22:R0:38:VAL:HG22 | 1.98 | 0.46 |
| 1:RA:140:G:N3 | 1:RA:142(A):A:N6 | 2.57 | 0.46 |
| 1:RA:2023:G:H4' | 1:RA:2617:C:O3' | 2.16 | 0.46 |
| 13:RR:44:LEU:HD22 | 13:RR:48:VAL:HG23 | 1.97 | 0.46 |
| 32:XA:520:A:N1 | 32:XA:536:C:H1' | 2.30 | 0.46 |
| 32:XA:736:C:H2' | 32:XA:737:A:C8 | 2.51 | 0.46 |
| 38:XG:27:ILE:HD12 | 38:XG:40:ALA:HA | 1.97 | 0.46 |
| 55:XY:227:PHE:O | 55:XY:243:ALA:HB3 | 2.16 | 0.46 |
| 1:YA:1053:C:O2' | 1:YA:1054:A:O5' | 2.34 | 0.46 |
| 1:YA:185:U:H4' | 1:YA:218:A:H4' | 1.98 | 0.46 |
| 1:YA:740:U:H2' | 1:YA:741:G:C8 | 2.50 | 0.46 |
| 1:YA:84:A:N1 | 1:YA:98:G:O2' | 2.42 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:YA:817:C:H4' | 1:YA:932:G:C5 | 2.51 | 0.46 |
| 32:QA:1003:G:C2 | 32:QA:1004:A:N3 | 2.84 | 0.46 |
| 52:QU:5:ASP:O | 52:QU:11:GLY:HA3 | 2.16 | 0.46 |
| 1:RA:1063:G:H2' | 1:RA:1065:U:H6 | 1.80 | 0.46 |
| 1:RA:10:G:H1' | 1:RA:2801(B):A:N1 | 2.31 | 0.46 |
| 1:RA:2693:A:H2' | 1:RA:2694:G:H8 | 1.80 | 0.46 |
| 1:RA:192:C:O2' | 1:RA:802:A:N3 | 2.42 | 0.46 |
| 15:RT:108:ARG:HA | 15:RT:111:ARG:NH1 | 2.30 | 0.46 |
| 44:XM:34:LEU:HD13 | 44:XM:41:PRO:HA | 1.98 | 0.46 |
| 1:YA:2564:A:C2 | 1:YA:2647:U:H4' | 2.51 | 0.46 |
| 1:YA:2741:A:OP1 | 31:Y9:22:ARG:NH2 | 2.42 | 0.46 |
| 1:YA:2754:U:O2' | 31:Y9:17:ILE:HG12 | 2.16 | 0.46 |
| 1:YA:247:G:H4' | 1:YA:386:G:C5 | 2.50 | 0.46 |
| 1:YA:492:A:H2' | 1:YA:493:G:O4' | 2.16 | 0.46 |
| 1:YA:668:G:H5' | 1:YA:669:G:OP2 | 2.15 | 0.46 |
| 1:YA:754:C:H2' | 1:YA:755:C:C6 | 2.51 | 0.46 |
| 10:YO:10:VAL:HG21 | 10:YO:16:ALA:HB3 | 1.97 | 0.46 |
| 12:YQ:109:VAL:HG13 | 12:YQ:113:GLN:HB2 | 1.97 | 0.46 |
| 32:QA:1053:G:N7 | 32:QA:1200:C:H5'' | 2.31 | 0.46 |
| 32:QA:828:A:H2' | 32:QA:829:G:O4' | 2.16 | 0.46 |
| 36:QE:31:LEU:HA | 36:QE:31:LEU:HD23 | 1.82 | 0.46 |
| 42:QK:34:ASP:OD2 | 42:QK:38:ASN:HB2 | 2.16 | 0.46 |
| 42:QK:92:GLU:O | 42:QK:96:ARG:HG2 | 2.16 | 0.46 |
| 1:RA:1581:G:H2' | 1:RA:1582:C:O4' | 2.15 | 0.46 |
| 6:RG:7:LEU:HD13 | 6:RG:100:TRP:HE3 | 1.81 | 0.46 |
| 1:RA:2012:G:OP1 | 18:RW:11:ARG:NH2 | 2.46 | 0.46 |
| 32:XA:1129:C:N4 | 32:XA:1143:G:H1 | 2.14 | 0.46 |
| 32:XA:1164:G:H1 | 32:XA:1172:C:N4 | 2.13 | 0.46 |
| 32:XA:1286:A:C8 | 32:XA:1287:A:H4' | 2.51 | 0.46 |
| 32:XA:262:A:H2' | 32:XA:263:A:C8 | 2.51 | 0.46 |
| 1:YA:277:C:H1' | 1:YA:278:A:OP1 | 2.15 | 0.46 |
| 1:YA:455:C:N3 | 1:YA:472:A:H2' | 2.30 | 0.46 |
| 2:YB:84:C:OP1 | 25:Y3:15:TYR:OH | 2.24 | 0.46 |
| 3:YD:5:LYS:HB3 | 3:YD:5:LYS:HE3 | 1.67 | 0.46 |
| 32:QA:1015:A:H2' | 32:QA:1016:A:C8 | 2.51 | 0.46 |
| 32:QA:1201:A:H1' | 32:QA:1202:G:OP2 | 2.16 | 0.46 |
| 32:QA:15:G:H1' | 36:QE:24:ARG:HE | 1.79 | 0.46 |
| 37:QF:76:ALA:O | 37:QF:80:ARG:HG3 | 2.16 | 0.46 |
| 32:QA:1343:G:H4' | 40:QI:122:ALA:HB3 | 1.98 | 0.46 |
| 55:QY:316:ARG:HG2 | 55:QY:327:TYR:CE2 | 2.51 | 0.46 |
| 1:RA:1587:A:H2' | 1:RA:1588:C:C6 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:RA:1790:C:H5'' | 1:RA:1791:A:OP1 | 2.15 | 0.46 |
| 1:RA:1693:U:O2' | 3:RD:14:ARG:NH2 | 2.48 | 0.46 |
| 3:RD:12:SER:HB3 | 3:RD:208:LYS:HB3 | 1.98 | 0.46 |
| 6:RG:50:ALA:C | 6:RG:52:ILE:N | 2.69 | 0.46 |
| 32:XA:1035:A:H2' | 32:XA:1036:G:C8 | 2.51 | 0.46 |
| 32:XA:767:A:H2' | 32:XA:768:A:O4' | 2.16 | 0.46 |
| 33:XB:48:MET:HA | 33:XB:51:LEU:HD12 | 1.98 | 0.46 |
| 50:XS:41:VAL:HG22 | 50:XS:42:PRO:HD2 | 1.97 | 0.46 |
| 55:XY:177:PHE:CA | 55:XY:321:ARG:HH22 | 2.29 | 0.46 |
| 1:YA:1899:G:N3 | 1:YA:1899:G:H2' | 2.31 | 0.46 |
| 1:YA:479:A:N3 | 1:YA:481:G:H5'' | 2.31 | 0.46 |
| 33:QB:134:GLU:HG3 | 33:QB:137:ARG:NH2 | 2.32 | 0.45 |
| 32:QA:427:U:OP1 | 35:QD:13:ARG:NH2 | 2.49 | 0.45 |
| 39:QH:82:HIS:NE2 | 39:QH:84:ARG:HG2 | 2.31 | 0.45 |
| 41:QJ:33:GLN:O | 41:QJ:75:ILE:N | 2.37 | 0.45 |
| 44:QM:81:LEU:HD13 | 44:QM:88:ARG:HG2 | 1.98 | 0.45 |
| 55:QY:133:ARG:NH1 | 55:QY:334:GLU:HG2 | 2.31 | 0.45 |
| 55:QY:236:HIS:CD2 | 55:QY:240:THR:HG21 | 2.51 | 0.45 |
| 55:QY:311:ASN:O | 55:QY:329:LEU:HD11 | 2.16 | 0.45 |
| 1:RA:1341:U:O4' | 19:RX:57:LEU:HD23 | 2.16 | 0.45 |
| 1:RA:2184:G:N1 | 1:RA:2185:C:O2 | 2.49 | 0.45 |
| 1:RA:2328:A:H2' | 1:RA:2329:G:C8 | 2.51 | 0.45 |
| 6:RG:181:ARG:HG3 | 6:RG:182:LYS:N | 2.31 | 0.45 |
| 11:RP:126:VAL:CG1 | 11:RP:148:LEU:HD21 | 2.46 | 0.45 |
| 32:XA:1028:C:H2' | 32:XA:1033:G:H22 | 1.81 | 0.45 |
| 32:XA:1101:A:H4' | 32:XA:1102:A:O5' | 2.16 | 0.45 |
| 32:XA:1279:A:O2' | 32:XA:1281:U:OP2 | 2.30 | 0.45 |
| 26:Y4:48:ARG:HB3 | 26:Y4:52:THR:HA | 1.98 | 0.45 |
| 11:YP:63:PRO:HG2 | 30:Y8:25:MET:HB2 | 1.98 | 0.45 |
| 1:YA:848:G:H2' | 1:YA:849:A:C8 | 2.51 | 0.45 |
| 6:YG:46:ALA:HB2 | 6:YG:53:LEU:HG | 1.97 | 0.45 |
| 16:YU:103:PRO:HD2 | 16:YU:104:GLN:NE2 | 2.30 | 0.45 |
| 17:YV:98:GLU:OE1 | 17:YV:100:ARG:NH1 | 2.50 | 0.45 |
| 32:QA:1304:G:OP1 | 52:QU:2:GLY:N | 2.49 | 0.45 |
| 35:QD:53:ASP:HB3 | 35:QD:57:ARG:NH1 | 2.30 | 0.45 |
| 40:QI:77:ILE:O | 40:QI:81:ILE:HG23 | 2.17 | 0.45 |
| 50:QS:22:LEU:HD12 | 50:QS:31:ILE:HD11 | 1.97 | 0.45 |
| 53:QV:17(A):U:H5'' | 53:QV:18:G:OP2 | 2.16 | 0.45 |
| 1:RA:1340:U:OP1 | 19:RX:16:LYS:NZ | 2.46 | 0.45 |
| 1:RA:2134:A:H8 | 1:RA:2156:G:H21 | 1.63 | 0.45 |
| 12:RQ:11:LYS:HE2 | 12:RQ:88:GLY:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:XA:1318:A:H5'' | 50:XS:3:ARG:NH2 | 2.30 | 0.45 |
| 33:XB:22:LYS:HE3 | 33:XB:22:LYS:HB2 | 1.73 | 0.45 |
| 1:YA:2279:G:O6 | 22:Y0:14:ARG:HD2 | 2.15 | 0.45 |
| 23:Y1:51:VAL:HG11 | 23:Y1:74:VAL:HG21 | 1.98 | 0.45 |
| 1:YA:1292:U:H2' | 1:YA:1293:C:C6 | 2.50 | 0.45 |
| 1:YA:1341:U:O4' | 19:YX:57:LEU:HD23 | 2.15 | 0.45 |
| 1:YA:1936:A:OP2 | 1:YA:1962:5MC:N4 | 2.43 | 0.45 |
| 1:YA:2106:G:C4 | 1:YA:2107:C:H1' | 2.51 | 0.45 |
| 1:YA:662:G:H5' | 11:YP:14:LYS:O | 2.16 | 0.45 |
| 3:YD:108:PRO:HG2 | 3:YD:111:LEU:HB2 | 1.98 | 0.45 |
| 7:YH:3:ARG:NH1 | 7:YH:3:ARG:HB3 | 2.31 | 0.45 |
| 20:YY:99:CYS:SG | 20:YY:100:ALA:N | 2.88 | 0.45 |
| 32:QA:1136:U:H5'' | 32:QA:1137:C:C2 | 2.51 | 0.45 |
| 32:QA:620:C:C2 | 35:QD:135:LEU:HG | 2.52 | 0.45 |
| 32:QA:657:G:H4' | 46:QO:28:GLN:HG2 | 1.98 | 0.45 |
| 32:QA:744:C:O2' | 32:QA:851:G:N2 | 2.48 | 0.45 |
| 39:QH:6:ILE:HB | 39:QH:85:ARG:NH1 | 2.30 | 0.45 |
| 32:QA:1226:C:N4 | 44:QM:104:ARG:HD2 | 2.31 | 0.45 |
| 25:R3:3:ARG:HH11 | 25:R3:60:GLU:CD | 2.19 | 0.45 |
| 26:R4:10:VAL:HG21 | 26:R4:29:PRO:HG3 | 1.99 | 0.45 |
| 1:RA:30:G:H2' | 1:RA:31:C:C6 | 2.50 | 0.45 |
| 5:RF:125:LEU:HD12 | 5:RF:194:MET:HB2 | 1.97 | 0.45 |
| 19:RX:60:ARG:NH2 | 29:R7:47:ARG:HH22 | 2.14 | 0.45 |
| 32:XA:848:C:H2' | 32:XA:849:C:H6 | 1.82 | 0.45 |
| 32:XA:946:A:H2' | 32:XA:947:G:C8 | 2.51 | 0.45 |
| 34:XC:19:GLU:HB3 | 34:XC:40:ARG:HH22 | 1.80 | 0.45 |
| 35:XD:190:ASP:O | 35:XD:193:ASP:HB2 | 2.16 | 0.45 |
| 49:XR:26:LEU:HD11 | 49:XR:42:ARG:NE | 2.31 | 0.45 |
| 24:Y2:21:LEU:HB2 | 24:Y2:64:LEU:HD23 | 1.98 | 0.45 |
| 26:Y4:40:HIS:HB3 | 26:Y4:43:TYR:CD1 | 2.51 | 0.45 |
| 1:YA:2311:A:H3' | 1:YA:2312:U:C6 | 2.52 | 0.45 |
| 19:YX:61:GLY:HA3 | 19:YX:73:ARG:O | 2.16 | 0.45 |
| 32:QA:1239:A:H62 | 32:QA:1299:A:N6 | 2.15 | 0.45 |
| 1:RA:1032:A:H4' | 31:R9:16:VAL:HG11 | 1.98 | 0.45 |
| 1:RA:108:U:H2' | 1:RA:109:G:C8 | 2.51 | 0.45 |
| 1:RA:1102:C:H2' | 1:RA:1103:A:C8 | 2.51 | 0.45 |
| 1:RA:2572:A:C8 | 4:RE:144:ARG:HG2 | 2.52 | 0.45 |
| 16:RU:108:GLU:O | 16:RU:112:ARG:HG2 | 2.16 | 0.45 |
| 32:XA:142:G:H2' | 32:XA:143:A:C8 | 2.49 | 0.45 |
| 35:XD:108:LEU:HB3 | 35:XD:110:PHE:CD1 | 2.52 | 0.45 |
| 35:XD:148:VAL:HG11 | 35:XD:158:ILE:HG21 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 40:XI:23:ASN:OD1 | 40:XI:25:LYS:HE3 | 2.17 | 0.45 |
| 54:XX:21:A:H62 | 55:XY:198:THR:HG1 | 1.64 | 0.45 |
| 1:YA:1051:G:H4' | 1:YA:2752:C:C4' | 2.44 | 0.45 |
| 1:YA:1070:A:H2' | 1:YA:1071:G:C8 | 2.52 | 0.45 |
| 1:YA:2061:G:H5'' | 1:YA:2503:2MA:C2 | 2.46 | 0.45 |
| 1:YA:2064:C:H2' | 1:YA:2065:C:C6 | 2.52 | 0.45 |
| 12:YQ:30:GLY:HA2 | 12:YQ:107:ALA:HB2 | 1.98 | 0.45 |
| 13:YR:33:ARG:NH1 | 13:YR:115:GLU:OE2 | 2.49 | 0.45 |
| 32:QA:123:C:OP1 | 32:QA:311:C:O2' | 2.27 | 0.45 |
| 33:QB:40:HIS:HB3 | 33:QB:190:THR:HG21 | 1.98 | 0.45 |
| 33:QB:44:LEU:HD12 | 33:QB:44:LEU:HA | 1.77 | 0.45 |
| 35:QD:108:LEU:HD12 | 35:QD:176:LEU:HD13 | 1.99 | 0.45 |
| 36:QE:102:ALA:HB1 | 36:QE:106:PRO:HG2 | 1.97 | 0.45 |
| 55:QY:111:ALA:HB2 | 55:QY:172:TYR:HB2 | 1.98 | 0.45 |
| 1:RA:1593:G:H2' | 1:RA:1594:G:C8 | 2.51 | 0.45 |
| 1:RA:2693:A:H2' | 1:RA:2694:G:C8 | 2.52 | 0.45 |
| 1:RA:323:G:H1' | 1:RA:1205:U:O2 | 2.16 | 0.45 |
| 1:RA:36:G:N3 | 1:RA:450:G:O2' | 2.48 | 0.45 |
| 4:RE:36:ARG:HG2 | 4:RE:47:VAL:HG22 | 1.98 | 0.45 |
| 6:RG:108:ASN:HA | 26:R4:37:SER:HB3 | 1.97 | 0.45 |
| 7:RH:117:PRO:HG3 | 7:RH:123:PHE:CD2 | 2.51 | 0.45 |
| 15:RT:39:ARG:NH1 | 15:RT:41:ARG:HD3 | 2.31 | 0.45 |
| 33:XB:87:ARG:HD3 | 33:XB:234:PRO:HD2 | 1.97 | 0.45 |
| 32:XA:235:C:H5' | 48:XQ:70:ARG:HG2 | 1.98 | 0.45 |
| 53:XV:43:A:H2' | 53:XV:44:A:C8 | 2.51 | 0.45 |
| 1:YA:2001:A:H2' | 1:YA:2002:G:C8 | 2.51 | 0.45 |
| 1:YA:2051:A:H5' | 1:YA:2578:G:O4' | 2.16 | 0.45 |
| 1:YA:910:A:C6 | 1:YA:911:A:C6 | 3.04 | 0.45 |
| 2:YB:17:C:H2' | 2:YB:18:G:O4' | 2.16 | 0.45 |
| 7:YH:86:GLU:OE2 | 7:YH:132:ARG:NH2 | 2.49 | 0.45 |
| 32:QA:1030(C):C:H2' | 32:QA:1030(C):C:O2 | 2.16 | 0.45 |
| 32:QA:12:U:H4' | 32:QA:526:C:H4' | 1.99 | 0.45 |
| 42:QK:62:GLN:HB2 | 42:QK:93:GLN:HG3 | 1.98 | 0.45 |
| 44:QM:4:ILE:HA | 44:QM:5:ALA:HA | 1.65 | 0.45 |
| 50:QS:3:ARG:NH1 | 50:QS:10:PHE:HB2 | 2.31 | 0.45 |
| 53:QV:76:A:H2' | 55:QY:234:GLY:HA3 | 1.99 | 0.45 |
| 55:QY:222:LEU:HD22 | 55:QY:246:ILE:HG22 | 1.98 | 0.45 |
| 1:RA:1053:C:H2' | 1:RA:1054:A:C8 | 2.46 | 0.45 |
| 1:RA:1097:U:H2' | 1:RA:1097:U:O2 | 2.15 | 0.45 |
| 1:RA:1049:C:H1' | 1:RA:1113:U:O2' | 2.17 | 0.45 |
| 1:RA:2092:U:H4' | 1:RA:2093:G:O5' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:RA:2243:U:H2' | 1:RA:2244:U:C6 | 2.51 | 0.45 |
| 1:RA:2364:C:H2' | 1:RA:2365:G:O4' | 2.16 | 0.45 |
| 1:RA:2466:C:H5'' | 31:R9:6:SER:HB3 | 1.99 | 0.45 |
| 15:RT:16:ARG:HD3 | 15:RT:18:ASP:OD1 | 2.17 | 0.45 |
| 15:RT:24:PRO:HD3 | 15:RT:52:ILE:HD12 | 1.99 | 0.45 |
| 32:XA:1005:A:H1' | 32:XA:1025:U:N3 | 2.32 | 0.45 |
| 32:XA:815:A:N7 | 32:XA:1509:C:O2' | 2.44 | 0.45 |
| 39:XH:19:VAL:HG23 | 39:XH:21:LYS:HD3 | 1.97 | 0.45 |
| 55:XY:229:SER:HB2 | 55:XY:237:VAL:HG13 | 1.99 | 0.45 |
| 29:Y7:10:ARG:NH1 | 29:Y7:14:LYS:HE3 | 2.31 | 0.45 |
| 1:YA:1005:C:H2' | 1:YA:1006:C:C6 | 2.52 | 0.45 |
| 1:YA:1084:A:C8 | 1:YA:1085:A:H4' | 2.52 | 0.45 |
| 1:YA:1050:A:H2 | 1:YA:2751:G:C2 | 2.33 | 0.45 |
| 4:YE:115:GLY:O | 4:YE:119:ARG:HB2 | 2.17 | 0.45 |
| 12:YQ:55:VAL:HG23 | 21:YZ:178:GLU:HB3 | 1.97 | 0.45 |
| 32:QA:1148:U:H2' | 32:QA:1149:C:O4' | 2.17 | 0.45 |
| 32:QA:1347:G:N2 | 32:QA:1373:G:H2' | 2.32 | 0.45 |
| 33:QB:7:VAL:HG12 | 33:QB:217:ARG:HD2 | 1.99 | 0.45 |
| 45:QN:27:CYS:SG | 45:QN:29:ARG:HB2 | 2.57 | 0.45 |
| 55:QY:236:HIS:NE2 | 55:QY:240:THR:HG21 | 2.32 | 0.45 |
| 1:RA:1932:A:H2' | 1:RA:1933:G:O4' | 2.17 | 0.45 |
| 1:RA:2061:G:H5'' | 1:RA:2503:2MA:C2 | 2.46 | 0.45 |
| 1:RA:852:G:H2' | 1:RA:853:G:C8 | 2.51 | 0.45 |
| 4:RE:111:ARG:HG2 | 4:RE:160:TYR:O | 2.17 | 0.45 |
| 15:RT:37:GLY:HA2 | 15:RT:38:ASN:HA | 1.69 | 0.45 |
| 32:XA:1068:G:H8 | 32:XA:1068:G:OP2 | 1.99 | 0.45 |
| 32:XA:580:U:H2' | 32:XA:581:G:O4' | 2.17 | 0.45 |
| 32:XA:67:C:H2' | 32:XA:68:G:C8 | 2.52 | 0.45 |
| 32:XA:814:A:H2' | 32:XA:816:A:H5'' | 1.98 | 0.45 |
| 1:YA:144:C:H5' | 19:YX:2:LYS:HE2 | 1.98 | 0.45 |
| 1:YA:700:G:O2' | 1:YA:1632:A:N3 | 2.44 | 0.45 |
| 1:YA:1916:A:H2' | 1:YA:1917:PSU:O4' | 2.16 | 0.45 |
| 1:YA:2298:A:N6 | 1:YA:2318:G:C8 | 2.83 | 0.45 |
| 1:YA:2298:A:N6 | 1:YA:2318:G:H8 | 2.15 | 0.45 |
| 2:YB:8:U:O2' | 14:YS:40:ILE:HD13 | 2.16 | 0.45 |
| 1:YA:1971:A:C4 | 3:YD:241:PRO:HD3 | 2.52 | 0.45 |
| 4:YE:101:ARG:CZ | 4:YE:171:GLU:HB2 | 2.47 | 0.45 |
| 8:YI:130:TYR:CE2 | 8:YI:132:PRO:HB3 | 2.52 | 0.45 |
| 32:QA:707:C:OP1 | 42:QK:85:ARG:NH1 | 2.49 | 0.45 |
| 37:QF:91:VAL:HG11 | 49:QR:72:ARG:NH1 | 2.31 | 0.45 |
| 39:QH:6:ILE:O | 39:QH:10:LEU:HG | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:QJ:19:SER:O | 41:QJ:23:ILE:HG12 | 2.17 | 0.45 |
| 48:QQ:58:GLU:OE2 | 48:QQ:75:ARG:NH2 | 2.50 | 0.45 |
| 30:R8:34:TRP:CE2 | 30:R8:35:GLN:HB3 | 2.51 | 0.45 |
| 1:RA:1153:C:H2' | 1:RA:1154:G:O4' | 2.17 | 0.45 |
| 1:RA:1557:C:H5'' | 1:RA:1558:A:OP2 | 2.17 | 0.45 |
| 1:RA:1847:A:H3' | 1:RA:1848:A:H5' | 1.99 | 0.45 |
| 1:RA:2031:A:N3 | 1:RA:2455:G:O2' | 2.38 | 0.45 |
| 1:RA:2107:C:H42 | 1:RA:2182:G:H1 | 1.65 | 0.45 |
| 1:RA:2128:C:H3' | 1:RA:2129:C:H5'' | 1.98 | 0.45 |
| 1:RA:2401:U:H3' | 1:RA:2402:C:C6 | 2.52 | 0.45 |
| 1:RA:2832:U:O4 | 1:RA:2883:A:H5'' | 2.17 | 0.45 |
| 11:RP:55:ARG:HG2 | 11:RP:56:SER:N | 2.31 | 0.45 |
| 17:RV:40:LEU:HB2 | 17:RV:46:VAL:HG12 | 1.97 | 0.45 |
| 33:XB:42:ILE:HD13 | 33:XB:203:GLY:HA2 | 1.98 | 0.45 |
| 51:XT:38:LYS:HE2 | 51:XT:38:LYS:HB3 | 1.68 | 0.45 |
| 1:YA:1049:C:H1' | 1:YA:1113:U:O2' | 2.16 | 0.45 |
| 1:YA:2023:G:H4' | 1:YA:2617:C:O3' | 2.17 | 0.45 |
| 1:YA:2516:G:C6 | 1:YA:2517:C:N4 | 2.85 | 0.45 |
| 1:YA:2849:U:H4' | 1:YA:2868:A:C2 | 2.51 | 0.45 |
| 1:YA:350:U:H2' | 1:YA:351:G:O4' | 2.17 | 0.45 |
| 1:YA:574:C:N3 | 4:YE:145:LYS:NZ | 2.45 | 0.45 |
| 4:YE:150:VAL:HG13 | 4:YE:154:LYS:HG3 | 1.98 | 0.45 |
| 7:YH:164:TYR:HB2 | 7:YH:167:GLU:HB2 | 1.98 | 0.45 |
| 32:QA:657:G:O2' | 46:QO:23:GLY:HA2 | 2.17 | 0.45 |
| 1:RA:1055:G:H2' | 1:RA:1056:G:O4' | 2.17 | 0.45 |
| 1:RA:1166:C:H2' | 1:RA:1167:U:C6 | 2.52 | 0.45 |
| 1:RA:1358:G:O2' | 1:RA:1359:A:H5' | 2.16 | 0.45 |
| 1:RA:2313:C:H2' | 1:RA:2314:C:C6 | 2.52 | 0.45 |
| 1:RA:2477:C:N4 | 31:R9:10:ILE:HG23 | 2.32 | 0.45 |
| 1:RA:1812:A:O2' | 3:RD:45:ASN:N | 2.49 | 0.45 |
| 32:XA:1154:G:H2' | 32:XA:1155:G:H8 | 1.82 | 0.45 |
| 32:XA:1327:C:H2' | 32:XA:1328:C:C6 | 2.52 | 0.45 |
| 32:XA:189(L):U:H2' | 32:XA:189(M):G:C8 | 2.52 | 0.45 |
| 38:XG:9:VAL:HG11 | 38:XG:94:ARG:HD3 | 1.98 | 0.45 |
| 41:XJ:38:ILE:CG1 | 41:XJ:71:LEU:HB3 | 2.47 | 0.45 |
| 32:XA:1492:A:C8 | 43:XL:47:LYS:HG2 | 2.51 | 0.45 |
| 51:XT:39:LYS:HB2 | 51:XT:39:LYS:HE3 | 1.80 | 0.45 |
| 53:XV:21:A:N6 | 53:XV:46:G:H2' | 2.32 | 0.45 |
| 1:YA:1029:A:C2 | 1:YA:2465:C:C2' | 3.00 | 0.45 |
| 1:YA:1097:U:H2' | 1:YA:1097:U:O2 | 2.15 | 0.45 |
| 1:YA:1358:G:O2' | 1:YA:1359:A:H5' | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:YA:2870:C:H2' | 1:YA:2871:C:O4' | 2.16 | 0.45 |
| 1:YA:458:G:O2' | 1:YA:469:G:O6 | 2.22 | 0.45 |
| 8:YI:4:ILE:HG12 | 8:YI:18:VAL:HG22 | 1.99 | 0.45 |
| 12:YQ:137:TYR:O | 12:YQ:141:GLN:HG2 | 2.17 | 0.45 |
| 32:QA:1058:G:OP1 | 34:QC:199:LYS:HE3 | 2.17 | 0.45 |
| 32:QA:1124:G:N7 | 32:QA:1145:C:O2' | 2.50 | 0.45 |
| 32:QA:262:A:H2' | 32:QA:263:A:C8 | 2.51 | 0.45 |
| 32:QA:309:G:O2' | 32:QA:607:A:N1 | 2.48 | 0.45 |
| 35:QD:173:TRP:CE3 | 35:QD:174:LEU:HG | 2.52 | 0.45 |
| 35:QD:85:LYS:HD3 | 35:QD:86:LYS:N | 2.31 | 0.45 |
| 38:QG:79:ARG:HA | 38:QG:84:ASN:HA | 1.98 | 0.45 |
| 1:RA:2317:C:H2' | 1:RA:2318:G:H5' | 1.99 | 0.45 |
| 32:XA:859:A:OP2 | 32:XA:869:G:N1 | 2.45 | 0.45 |
| 37:XF:100:ASN:ND2 | 49:XR:23:LYS:HE2 | 2.32 | 0.45 |
| 53:XV:47:U:H3' | 53:XV:48:C:C5' | 2.46 | 0.45 |
| 29:Y7:34:ARG:NH1 | 29:Y7:41:ARG:O | 2.50 | 0.45 |
| 1:YA:1794:U:H2' | 1:YA:1795:C:H6 | 1.81 | 0.45 |
| 1:YA:1939:5MU:OP1 | 1:YA:2604:U:O2' | 2.33 | 0.45 |
| 1:YA:2074:U:H2' | 1:YA:2075:U:C6 | 2.52 | 0.45 |
| 1:YA:2774:C:H2' | 1:YA:2775:A:O4' | 2.16 | 0.45 |
| 8:YI:40:THR:O | 8:YI:44:LEU:HD22 | 2.17 | 0.45 |
| 10:YO:120:GLU:HG2 | 10:YO:122:LEU:HG | 1.98 | 0.45 |
| 10:YO:9:GLU:O | 10:YO:83:ALA:HA | 2.17 | 0.45 |
| 16:YU:36:ARG:HD2 | 16:YU:40:PHE:CZ | 2.52 | 0.45 |
| 32:QA:1034:G:H3' | 32:QA:1035:A:C8 | 2.51 | 0.44 |
| 32:QA:1148:U:O3' | 40:QL:14:VAL:HG11 | 2.17 | 0.44 |
| 1:RA:2629:A:H1' | 1:RA:2630:G:H5'' | 1.99 | 0.44 |
| 1:RA:686:G:N2 | 1:RA:788:A:H61 | 2.15 | 0.44 |
| 1:RA:272(K):U:O2 | 8:RI:50:ARG:HD3 | 2.16 | 0.44 |
| 19:RX:60:ARG:HH12 | 29:R7:47:ARG:HH22 | 1.65 | 0.44 |
| 32:XA:434:U:H2' | 32:XA:435:C:C6 | 2.51 | 0.44 |
| 34:XC:43:LEU:O | 34:XC:47:LEU:HB2 | 2.16 | 0.44 |
| 35:XD:20:TYR:CD2 | 35:XD:26:CYS:HB3 | 2.52 | 0.44 |
| 36:XE:20:GLN:OE1 | 36:XE:25:ARG:HD2 | 2.17 | 0.44 |
| 37:XF:25:ILE:HD13 | 37:XF:82:ARG:HE | 1.82 | 0.44 |
| 42:XK:78:GLN:O | 42:XK:103:LEU:HA | 2.17 | 0.44 |
| 47:XP:43:LYS:HA | 47:XP:48:TRP:HB3 | 1.98 | 0.44 |
| 23:Y1:3:LYS:HB2 | 23:Y1:61:ARG:HH12 | 1.81 | 0.44 |
| 25:Y3:23:LEU:HD12 | 25:Y3:28:LEU:HB2 | 1.99 | 0.44 |
| 1:YA:1084:A:H3' | 1:YA:1085:A:H4' | 1.99 | 0.44 |
| 1:YA:11:G:C2' | 1:YA:12:U:H5' | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:YA:2629:A:H1' | 1:YA:2630:G:H5'' | 1.99 | 0.44 |
| 1:YA:523:C:H4' | 1:YA:540:C:O2 | 2.17 | 0.44 |
| 4:YE:11:MET:CG | 4:YE:24:THR:HG22 | 2.43 | 0.44 |
| 8:YI:69:LYS:HB2 | 8:YI:138:ILE:HG12 | 1.98 | 0.44 |
| 8:YI:6:LEU:HD11 | 8:YI:37:VAL:HG23 | 2.00 | 0.44 |
| 33:QB:41:ILE:HA | 33:QB:41:ILE:HD13 | 1.84 | 0.44 |
| 40:QI:22:GLY:HA3 | 40:QI:60:ASP:OD1 | 2.17 | 0.44 |
| 29:R7:24:THR:HG22 | 29:R7:27:GLY:H | 1.82 | 0.44 |
| 1:RA:2115:G:N2 | 1:RA:2171:A:H61 | 2.14 | 0.44 |
| 1:RA:2315:G:H2' | 1:RA:2316:C:C6 | 2.52 | 0.44 |
| 1:RA:764:A:O4' | 3:RD:213:ARG:HG3 | 2.17 | 0.44 |
| 4:RE:119:ARG:HG2 | 4:RE:120:TRP:CD1 | 2.52 | 0.44 |
| 32:XA:1159:U:O4' | 32:XA:1182:G:N2 | 2.50 | 0.44 |
| 32:XA:692:U:H1' | 32:XA:695:A:N7 | 2.32 | 0.44 |
| 44:XM:16:ASP:OD1 | 44:XM:16:ASP:N | 2.49 | 0.44 |
| 1:YA:1416:G:O2' | 1:YA:1417:C:OP2 | 2.29 | 0.44 |
| 1:YA:1472:A:H2' | 1:YA:1473:G:O4' | 2.17 | 0.44 |
| 1:YA:2016:U:H1' | 27:Y5:6:VAL:HG13 | 1.98 | 0.44 |
| 1:YA:2317:C:H2' | 1:YA:2318:G:H5' | 1.98 | 0.44 |
| 1:YA:2839:G:H5' | 13:YR:46:GLY:CA | 2.46 | 0.44 |
| 11:YP:106:LEU:HD13 | 11:YP:107:LYS:O | 2.17 | 0.44 |
| 1:YA:863:A:P | 12:YQ:22:LYS:HG3 | 2.58 | 0.44 |
| 32:QA:1179:A:H2' | 32:QA:1180:A:O4' | 2.17 | 0.44 |
| 33:QB:185:ILE:HG22 | 33:QB:199:TYR:HD2 | 1.80 | 0.44 |
| 35:QD:108:LEU:HB3 | 35:QD:110:PHE:CD1 | 2.53 | 0.44 |
| 36:QE:69:VAL:HG12 | 36:QE:139:LEU:HB3 | 1.98 | 0.44 |
| 39:QH:51:VAL:HG21 | 39:QH:60:ARG:HH11 | 1.81 | 0.44 |
| 39:QH:51:VAL:HG11 | 39:QH:60:ARG:HH12 | 1.83 | 0.44 |
| 45:QN:4:LYS:O | 45:QN:7:ILE:HG12 | 2.18 | 0.44 |
| 46:QO:18:PHE:HB2 | 46:QO:19:PRO:HD2 | 1.99 | 0.44 |
| 32:QA:1456:G:C2 | 51:QT:55:ILE:HD11 | 2.53 | 0.44 |
| 26:R4:24:THR:OG1 | 26:R4:25:TYR:N | 2.51 | 0.44 |
| 1:RA:1025:G:C4 | 1:RA:1135:C:H1' | 2.52 | 0.44 |
| 1:RA:1092:C:H6 | 1:RA:1092:C:OP2 | 2.00 | 0.44 |
| 1:RA:2277:G:OP2 | 22:R0:10:THR:HG21 | 2.17 | 0.44 |
| 1:RA:528:A:O2' | 1:RA:529:A:H5' | 2.17 | 0.44 |
| 1:RA:754:C:H2' | 1:RA:755:C:C6 | 2.52 | 0.44 |
| 1:RA:911:A:H2' | 12:RQ:9:TYR:OH | 2.17 | 0.44 |
| 1:RA:2786:U:O2' | 4:RE:62:PRO:O | 2.30 | 0.44 |
| 1:RA:470:A:OP1 | 5:RF:59:TYR:HE1 | 2.01 | 0.44 |
| 32:XA:1148:U:O2' | 40:XI:66:ARG:NH1 | 2.44 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:XB:212:GLN:OE1 | 33:XB:235:SER:OG | 2.32 | 0.44 |
| 55:XY:308:ARG:NH2 | 55:XY:319:ASP:OD2 | 2.25 | 0.44 |
| 1:YA:1104:C:H2' | 1:YA:1105:U:H6 | 1.81 | 0.44 |
| 1:YA:1408:C:C2 | 1:YA:1595:G:N2 | 2.85 | 0.44 |
| 1:YA:2119:A:H61 | 1:YA:2168:G:H21 | 1.66 | 0.44 |
| 1:YA:2704:C:H2' | 1:YA:2705:A:O4' | 2.17 | 0.44 |
| 32:QA:17:U:O2' | 32:QA:1079:G:H1' | 2.17 | 0.44 |
| 32:QA:393:A:H5' | 32:QA:483:C:O2' | 2.18 | 0.44 |
| 46:QO:26:GLU:HG3 | 46:QO:81:LEU:HD22 | 1.99 | 0.44 |
| 46:QO:82:ILE:O | 46:QO:86:GLY:N | 2.50 | 0.44 |
| 29:R7:12:ARG:NH2 | 29:R7:44:PRO:HB3 | 2.33 | 0.44 |
| 1:RA:2420:C:OP1 | 30:R8:34:TRP:HB3 | 2.18 | 0.44 |
| 1:RA:1406:U:H2' | 1:RA:1407:C:C6 | 2.52 | 0.44 |
| 1:RA:1639:U:C2' | 1:RA:1640:C:H5'' | 2.47 | 0.44 |
| 1:RA:2375:G:O2' | 1:RA:2377:A:N7 | 2.46 | 0.44 |
| 1:RA:2805:G:H2' | 1:RA:2807:G:H8 | 1.83 | 0.44 |
| 1:RA:580:C:H2' | 1:RA:581:C:C6 | 2.52 | 0.44 |
| 3:RD:10:THR:OG1 | 3:RD:13:ARG:HG2 | 2.16 | 0.44 |
| 32:XA:1403:C:H1' | 32:XA:1500:A:N1 | 2.33 | 0.44 |
| 32:XA:359:U:H2' | 32:XA:360:A:C8 | 2.53 | 0.44 |
| 32:XA:881:G:OP2 | 43:XL:12:ARG:NH2 | 2.51 | 0.44 |
| 35:XD:8:VAL:HG22 | 35:XD:21:LEU:HD13 | 1.97 | 0.44 |
| 44:XM:15:VAL:HG12 | 44:XM:45:VAL:HG22 | 1.99 | 0.44 |
| 53:XV:21:A:H61 | 53:XV:46:G:H2' | 1.82 | 0.44 |
| 55:XY:103:LYS:HG2 | 55:XY:103:LYS:H | 1.60 | 0.44 |
| 1:YA:1239:G:H2' | 1:YA:1240:U:O4' | 2.17 | 0.44 |
| 1:YA:2648:C:H2' | 1:YA:2649:U:C6 | 2.52 | 0.44 |
| 1:YA:2832:U:O4 | 1:YA:2883:A:H5'' | 2.17 | 0.44 |
| 2:YB:96:U:H2' | 2:YB:97:G:C8 | 2.53 | 0.44 |
| 1:YA:2680:C:H5' | 4:YE:189:PRO:HA | 2.00 | 0.44 |
| 15:YT:91:ARG:HD2 | 15:YT:120:ARG:NH1 | 2.32 | 0.44 |
| 19:YX:12:VAL:HG22 | 19:YX:29:TRP:CE2 | 2.52 | 0.44 |
| 32:QA:1333:A:H2' | 32:QA:1334:G:O4' | 2.18 | 0.44 |
| 32:QA:149:A:H2' | 32:QA:150:C:C6 | 2.52 | 0.44 |
| 40:QI:65:VAL:HG21 | 40:QI:73:GLN:HB3 | 2.00 | 0.44 |
| 32:QA:656:C:O2' | 46:QO:28:GLN:OE1 | 2.21 | 0.44 |
| 55:QY:318:THR:HG22 | 55:QY:325:THR:HB | 2.00 | 0.44 |
| 1:RA:1794:U:H2' | 1:RA:1795:C:H6 | 1.81 | 0.44 |
| 1:RA:1796:U:H2' | 1:RA:1797:C:H6 | 1.81 | 0.44 |
| 1:RA:1916:A:H2' | 1:RA:1917:PSU:O4' | 2.17 | 0.44 |
| 1:RA:2512:C:H2' | 1:RA:2513:G:O4' | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:RA:875:G:H2' | 1:RA:876:C:O4' | 2.18 | 0.44 |
| 5:RF:110:LEU:HA | 5:RF:183:VAL:HG12 | 1.99 | 0.44 |
| 20:RY:9:LYS:HA | 20:RY:10:GLY:HA2 | 1.74 | 0.44 |
| 32:XA:1005:A:H1' | 32:XA:1025:U:C2 | 2.52 | 0.44 |
| 32:XA:397:A:H3' | 32:XA:397:A:N3 | 2.32 | 0.44 |
| 35:XD:191:ARG:HA | 35:XD:191:ARG:HD2 | 1.76 | 0.44 |
| 47:XP:18:ARG:NH1 | 47:XP:32:TYR:OH | 2.51 | 0.44 |
| 50:XS:12:ASP:OD2 | 50:XS:35:SER:HB3 | 2.17 | 0.44 |
| 55:XY:213:GLU:C | 55:XY:215:PRO:HD3 | 2.38 | 0.44 |
| 1:YA:1069:A:H5' | 1:YA:1096:A:C5' | 2.48 | 0.44 |
| 1:YA:9:U:O2' | 1:YA:10:G:OP1 | 2.32 | 0.44 |
| 1:YA:1102:C:H2' | 1:YA:1103:A:C8 | 2.52 | 0.44 |
| 1:YA:93:G:H2' | 1:YA:94(A):C:C6 | 2.53 | 0.44 |
| 8:YI:62:LYS:HG2 | 8:YI:133:HIS:NE2 | 2.33 | 0.44 |
| 16:YU:92:ARG:HA | 16:YU:95:LEU:HB2 | 1.98 | 0.44 |
| 32:QA:864:A:H2' | 32:QA:865:A:C8 | 2.52 | 0.44 |
| 33:QB:185:ILE:HG22 | 33:QB:199:TYR:CD2 | 2.53 | 0.44 |
| 33:QB:8:LYS:HZ3 | 33:QB:52:GLU:HB2 | 1.83 | 0.44 |
| 34:QC:22:TRP:CD1 | 34:QC:59:ARG:HD2 | 2.52 | 0.44 |
| 35:QD:194:LEU:HD12 | 35:QD:195:ALA:H | 1.82 | 0.44 |
| 32:QA:406:G:H5' | 35:QD:5:ILE:HD11 | 1.99 | 0.44 |
| 40:QI:16:ARG:HH11 | 40:QI:64:THR:HG21 | 1.83 | 0.44 |
| 26:R4:15:ILE:HB | 26:R4:32:TYR:CD1 | 2.53 | 0.44 |
| 1:RA:1011:G:H1' | 1:RA:1013:C:O4' | 2.18 | 0.44 |
| 1:RA:1104:C:H2' | 1:RA:1105:U:H6 | 1.83 | 0.44 |
| 1:RA:2016:U:H1' | 27:R5:6:VAL:HG13 | 1.98 | 0.44 |
| 20:RY:90:LEU:HD21 | 20:RY:96:ILE:HG12 | 1.99 | 0.44 |
| 32:XA:266:G:H5'' | 32:XA:266:G:N3 | 2.33 | 0.44 |
| 32:XA:992:U:H4' | 32:XA:993:G:C5' | 2.48 | 0.44 |
| 34:XC:63:ASN:HB2 | 34:XC:98:ASN:HB2 | 1.99 | 0.44 |
| 49:XR:21:LYS:HA | 49:XR:21:LYS:HD3 | 1.79 | 0.44 |
| 1:YA:1045:A:N3 | 1:YA:1045:A:H2' | 2.33 | 0.44 |
| 1:YA:1164:G:H2' | 1:YA:1165:U:C6 | 2.52 | 0.44 |
| 1:YA:1400:G:H2' | 1:YA:1401:G:C8 | 2.53 | 0.44 |
| 1:YA:195:A:H61 | 1:YA:198:C:H3' | 1.83 | 0.44 |
| 1:YA:2320:A:N3 | 1:YA:2320:A:H2' | 2.33 | 0.44 |
| 5:YF:20:LEU:HD12 | 5:YF:125:LEU:HD13 | 2.00 | 0.44 |
| 13:YR:56:LYS:NZ | 13:YR:90:ARG:O | 2.51 | 0.44 |
| 32:QA:1070:U:H2' | 32:QA:1071:C:H6 | 1.83 | 0.44 |
| 32:QA:956:U:OP2 | 55:QY:137:ARG:NH2 | 2.51 | 0.44 |
| 33:QB:9:GLU:CD | 33:QB:217:ARG:HH22 | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:QF:25:ILE:HG13 | 37:QF:82:ARG:HH12 | 1.81 | 0.44 |
| 38:QG:111:ARG:HB3 | 38:QG:113:GLU:OE2 | 2.17 | 0.44 |
| 38:QG:45:ASP:O | 38:QG:49:ILE:HG13 | 2.18 | 0.44 |
| 42:QK:85:ARG:HD3 | 42:QK:113:PRO:HD3 | 2.00 | 0.44 |
| 51:QT:57:ARG:NH1 | 51:QT:100:ILE:HD12 | 2.31 | 0.44 |
| 1:RA:1309:G:P | 29:R7:9:ARG:HD3 | 2.58 | 0.44 |
| 1:RA:1041:C:N4 | 1:RA:1114:G:H1 | 2.04 | 0.44 |
| 1:RA:1514:U:H2' | 1:RA:1515:G:C8 | 2.53 | 0.44 |
| 1:RA:1827:C:O2' | 1:RA:1970:A:N3 | 2.41 | 0.44 |
| 1:RA:2133:G:N2 | 1:RA:2157:G:H2' | 2.33 | 0.44 |
| 1:RA:2152:G:H2' | 1:RA:2153:G:H8 | 1.81 | 0.44 |
| 1:RA:2228:G:OP1 | 3:RD:261:LYS:NZ | 2.29 | 0.44 |
| 1:RA:2331:G:O2' | 1:RA:2336:A:N1 | 2.41 | 0.44 |
| 32:XA:1239:A:C4 | 32:XA:1298:C:N4 | 2.86 | 0.44 |
| 32:XA:1244:C:H2' | 32:XA:1245:A:C8 | 2.53 | 0.44 |
| 32:XA:1266:G:N2 | 32:XA:1269:A:OP2 | 2.46 | 0.44 |
| 32:XA:297:G:H4' | 32:XA:557:G:H4' | 1.99 | 0.44 |
| 33:XB:53:ARG:HG2 | 33:XB:56:ARG:HH21 | 1.83 | 0.44 |
| 44:XM:13:LYS:HA | 44:XM:44:ARG:HH11 | 1.82 | 0.44 |
| 48:XQ:81:ARG:HD2 | 48:XQ:81:ARG:HA | 1.81 | 0.44 |
| 32:XA:1492:A:C2' | 55:XY:303:ARG:HH12 | 2.31 | 0.44 |
| 3:YD:71:ASP:HB3 | 3:YD:103:ARG:NH2 | 2.32 | 0.44 |
| 3:YD:85:ASP:OD2 | 3:YD:88:ARG:HD2 | 2.18 | 0.44 |
| 1:YA:1143:A:OP1 | 9:YN:25:ARG:NH2 | 2.51 | 0.44 |
| 32:QA:1158:C:H5 | 32:QA:1181:G:N1 | 2.16 | 0.44 |
| 32:QA:179:A:H2' | 32:QA:180:U:H6 | 1.83 | 0.44 |
| 32:QA:520:A:N1 | 32:QA:536:C:H1' | 2.33 | 0.44 |
| 32:QA:1071:C:H5'' | 36:QE:49:PRO:HG2 | 1.99 | 0.44 |
| 41:QJ:11:PHE:CE1 | 41:QJ:67:THR:HG22 | 2.48 | 0.44 |
| 43:QL:33:ARG:NH1 | 43:QL:62:SER:HB3 | 2.33 | 0.44 |
| 44:QM:15:VAL:O | 44:QM:19:LEU:HD13 | 2.18 | 0.44 |
| 1:RA:1027:A:C6 | 1:RA:1126:A:C4 | 3.06 | 0.44 |
| 1:RA:2823:A:OP1 | 4:RE:113:PHE:HB2 | 2.18 | 0.44 |
| 1:RA:634:C:H2' | 1:RA:635:C:C6 | 2.53 | 0.44 |
| 3:RD:5:LYS:HB3 | 3:RD:5:LYS:HE3 | 1.82 | 0.44 |
| 40:XI:26:VAL:HG13 | 40:XI:61:ALA:HB3 | 1.99 | 0.44 |
| 55:XY:123:GLU:OE2 | 55:XY:186:ARG:HD3 | 2.18 | 0.44 |
| 24:Y2:35:LEU:HD21 | 24:Y2:49:LYS:HE2 | 2.00 | 0.44 |
| 1:YA:1410:G:H2' | 1:YA:1411:C:C6 | 2.53 | 0.44 |
| 1:YA:2107:C:H42 | 1:YA:2182:G:H1 | 1.66 | 0.44 |
| 1:YA:362:U:O2' | 1:YA:363(A):G:H5' | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:YA:721:C:H2' | 1:YA:722:A:C8 | 2.53 | 0.44 |
| 12:YQ:52:VAL:HA | 12:YQ:55:VAL:HG12 | 1.99 | 0.44 |
| 32:QA:1241:G:H2' | 32:QA:1242:C:C6 | 2.53 | 0.44 |
| 32:QA:131:C:H2' | 32:QA:132:C:C6 | 2.52 | 0.44 |
| 32:QA:134:A:H61 | 47:QP:25:ARG:NH1 | 2.16 | 0.44 |
| 32:QA:19:C:O2' | 32:QA:572:A:N1 | 2.42 | 0.44 |
| 33:QB:155:LEU:HD11 | 33:QB:159:PRO:HD3 | 2.00 | 0.44 |
| 34:QC:180:ALA:HB1 | 34:QC:203:PHE:CE1 | 2.52 | 0.44 |
| 44:QM:16:ASP:N | 44:QM:16:ASP:OD1 | 2.49 | 0.44 |
| 26:R4:7:PRO:HB2 | 26:R4:27:THR:HG21 | 1.99 | 0.44 |
| 1:RA:1210:A:H4' | 1:RA:1211:U:O5' | 2.17 | 0.44 |
| 1:RA:2893:G:H5'' | 1:RA:2894:G:O4' | 2.18 | 0.44 |
| 1:RA:881:G:H2' | 1:RA:882:G:C8 | 2.52 | 0.44 |
| 8:RI:85:GLU:HB3 | 8:RI:86:THR:H | 1.59 | 0.44 |
| 15:RT:51:ARG:HG3 | 15:RT:98:LYS:HE3 | 1.99 | 0.44 |
| 32:XA:1414:U:H3 | 32:XA:1486:G:H1 | 1.65 | 0.44 |
| 32:XA:738:C:OP1 | 37:XF:2:ARG:NH1 | 2.48 | 0.44 |
| 23:Y1:83:GLU:HA | 23:Y1:84:GLY:HA2 | 1.66 | 0.44 |
| 1:YA:1941:C:C5 | 1:YA:1942:5MC:HM52 | 2.53 | 0.44 |
| 1:YA:2128:C:H3' | 1:YA:2129:C:H5'' | 2.00 | 0.44 |
| 1:YA:2552:2MU:H2' | 1:YA:2554:U:OP2 | 2.18 | 0.44 |
| 1:YA:2687:U:H2' | 1:YA:2688:U:O4' | 2.18 | 0.44 |
| 1:YA:2889:C:H3' | 1:YA:2891:G:C8 | 2.53 | 0.44 |
| 2:YB:95:C:H2' | 2:YB:96:U:C6 | 2.53 | 0.44 |
| 7:YH:95:ARG:HB2 | 7:YH:128:PRO:HB3 | 1.99 | 0.44 |
| 11:YP:135:LEU:HA | 11:YP:135:LEU:HD23 | 1.72 | 0.44 |
| 14:YS:43:GLU:OE1 | 22:Y0:49:LYS:HE3 | 2.17 | 0.44 |
| 32:QA:1024:G:N2 | 32:QA:1025:U:O4' | 2.48 | 0.43 |
| 32:QA:134:A:H1' | 32:QA:325:A:C5 | 2.53 | 0.43 |
| 32:QA:977:A:H1' | 32:QA:982:U:O4 | 2.18 | 0.43 |
| 40:QI:24:GLY:HA2 | 40:QI:59:PHE:O | 2.18 | 0.43 |
| 1:RA:531:C:H4' | 1:RA:532:A:H5'' | 2.00 | 0.43 |
| 32:XA:1030(B):G:O5' | 32:XA:1030(B):G:H8 | 2.01 | 0.43 |
| 32:XA:1347:G:HO2' | 32:XA:1373:G:H1 | 1.64 | 0.43 |
| 32:XA:501:C:OP1 | 43:XL:117:ARG:NH2 | 2.33 | 0.43 |
| 32:XA:790:A:C6 | 32:XA:791:G:C6 | 3.06 | 0.43 |
| 1:YA:1110:G:H1' | 1:YA:1111:A:H8 | 1.82 | 0.43 |
| 1:YA:2149:G:C2 | 1:YA:2150:U:H1' | 2.53 | 0.43 |
| 1:YA:2286:A:H4' | 1:YA:2287:A:O4' | 2.18 | 0.43 |
| 1:YA:251:A:C5 | 1:YA:252:G:H1' | 2.53 | 0.43 |
| 1:YA:2689:U:P | 1:YA:2719:G:H22 | 2.41 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:394:A:C6 | 1:YA:395:U:C4 | 3.06 | 0.43 |
| 1:YA:1500:G:O2' | 3:YD:100:GLY:O | 2.32 | 0.43 |
| 14:YS:25:ARG:HD3 | 14:YS:42:ASP:OD2 | 2.18 | 0.43 |
| 32:QA:161:A:H8 | 32:QA:161:A:O5' | 2.01 | 0.43 |
| 33:QB:109:SER:O | 33:QB:112:VAL:HG22 | 2.18 | 0.43 |
| 53:QV:3:C:C2' | 53:QV:4:G:H5' | 2.48 | 0.43 |
| 55:QY:138:TYR:CD1 | 55:QY:336:LYS:HB2 | 2.54 | 0.43 |
| 1:RA:108:U:H2' | 1:RA:109:G:H8 | 1.83 | 0.43 |
| 1:RA:1378:A:OP1 | 29:R7:10:ARG:NH2 | 2.52 | 0.43 |
| 1:RA:93:G:H2' | 1:RA:94(A):C:C6 | 2.53 | 0.43 |
| 12:RQ:75:THR:HG21 | 12:RQ:87:LYS:HG2 | 1.99 | 0.43 |
| 32:XA:575:G:O2' | 32:XA:821:G:H5' | 2.18 | 0.43 |
| 32:XA:952:U:H4' | 32:XA:964:A:N1 | 2.33 | 0.43 |
| 33:XB:179:LYS:HA | 39:XH:72:PRO:HG3 | 2.00 | 0.43 |
| 38:XG:16:LEU:HD11 | 40:XI:45:ALA:HB2 | 2.00 | 0.43 |
| 32:XA:1202:G:H1' | 45:YN:29:ARG:HD2 | 2.00 | 0.43 |
| 37:XF:91:VAL:HG11 | 49:XR:72:ARG:NH1 | 2.33 | 0.43 |
| 55:XY:263:GLN:O | 55:XY:267:LYS:N | 2.48 | 0.43 |
| 1:YA:1429:G:H2' | 1:YA:1430:C:C6 | 2.53 | 0.43 |
| 1:YA:706:A:H2' | 1:YA:707:G:O4' | 2.18 | 0.43 |
| 2:YB:14:U:O3' | 2:YB:108:U:O2' | 2.33 | 0.43 |
| 4:YE:119:ARG:HD3 | 4:YE:160:TYR:HB2 | 2.00 | 0.43 |
| 5:YF:101:LEU:HD12 | 5:YF:102:PRO:HD2 | 2.00 | 0.43 |
| 6:YG:170:ARG:HH21 | 6:YG:180:PHE:CB | 2.31 | 0.43 |
| 1:YA:2311:A:C2 | 6:YG:80:PHE:HB3 | 2.53 | 0.43 |
| 7:YH:137:ASP:HB3 | 7:YH:140:LYS:HB3 | 2.01 | 0.43 |
| 7:YH:33:LEU:HD11 | 7:YH:75:ALA:HB1 | 2.00 | 0.43 |
| 35:QD:15:GLU:OE2 | 35:QD:66:ARG:NH1 | 2.51 | 0.43 |
| 46:QO:71:GLN:HB2 | 46:QO:78:TYR:CG | 2.54 | 0.43 |
| 42:QK:109:VAL:HG23 | 49:QR:85:LEU:O | 2.18 | 0.43 |
| 1:RA:1472:A:H2' | 1:RA:1473:G:O4' | 2.18 | 0.43 |
| 1:RA:1423:G:OP1 | 1:RA:1492:G:O2' | 2.35 | 0.43 |
| 1:RA:2543:G:H2' | 1:RA:2544:G:C8 | 2.52 | 0.43 |
| 1:RA:2869:G:H2' | 1:RA:2870:C:O4' | 2.18 | 0.43 |
| 7:RH:137:ASP:HB3 | 7:RH:140:LYS:HB3 | 2.00 | 0.43 |
| 13:RR:24:GLN:HE21 | 13:RR:44:LEU:HG | 1.82 | 0.43 |
| 32:XA:1346:A:N1 | 32:XA:1374:A:H5'' | 2.32 | 0.43 |
| 32:XA:176:C:H2' | 32:XA:177:C:C6 | 2.54 | 0.43 |
| 32:XA:601:C:H2' | 32:XA:602:A:C8 | 2.53 | 0.43 |
| 32:XA:757:U:H2' | 32:XA:758:G:O4' | 2.19 | 0.43 |
| 33:XB:114:ARG:NH1 | 33:XB:118:LEU:HG | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:XB:18:GLY:HA2 | 33:XB:42:ILE:HD12 | 1.99 | 0.43 |
| 34:XC:137:ALA:HA | 34:XC:140:ARG:NH1 | 2.34 | 0.43 |
| 55:XY:121:GLY:O | 55:XY:123:GLU:N | 2.49 | 0.43 |
| 55:XY:177:PHE:CB | 55:XY:321:ARG:HH22 | 2.30 | 0.43 |
| 1:YA:1410:G:H1 | 1:YA:1592:C:H42 | 1.65 | 0.43 |
| 1:YA:1587:A:H2' | 1:YA:1588:C:C6 | 2.53 | 0.43 |
| 1:YA:2080:G:OP1 | 23:Y1:35:THR:HG21 | 2.18 | 0.43 |
| 1:YA:2186:G:C2 | 1:YA:2187:G:C5 | 3.06 | 0.43 |
| 1:YA:300:A:P | 20:YY:86:ARG:HH21 | 2.41 | 0.43 |
| 1:YA:309:G:H21 | 1:YA:330:A:P | 2.40 | 0.43 |
| 32:QA:1239:A:C4 | 32:QA:1298:C:N4 | 2.86 | 0.43 |
| 51:QT:39:LYS:HB2 | 51:QT:39:LYS:HE3 | 1.90 | 0.43 |
| 55:QY:123:GLU:HG3 | 55:QY:188:PRO:HB3 | 2.00 | 0.43 |
| 11:RP:62:LEU:O | 30:R8:13:ARG:HD3 | 2.19 | 0.43 |
| 1:RA:1704:G:H5' | 32:QA:1429:C:O2' | 2.17 | 0.43 |
| 1:RA:2130:U:H2' | 1:RA:2158:A:H61 | 1.83 | 0.43 |
| 1:RA:2130:U:H2' | 1:RA:2158:A:N1 | 2.34 | 0.43 |
| 18:RW:33:ARG:NH2 | 18:RW:52:GLU:OE1 | 2.50 | 0.43 |
| 32:XA:926:G:H22 | 54:XX:15:A:H3' | 1.83 | 0.43 |
| 34:XC:70:VAL:HG22 | 34:XC:72:LYS:H | 1.84 | 0.43 |
| 35:XD:122:ARG:NH1 | 35:XD:136:PRO:HD3 | 2.34 | 0.43 |
| 42:XK:116:HIS:N | 42:XK:117:ASN:HA | 2.34 | 0.43 |
| 47:XP:20:VAL:HG21 | 47:XP:32:TYR:CD2 | 2.53 | 0.43 |
| 49:XR:58:LEU:HD12 | 49:XR:62:GLU:CG | 2.48 | 0.43 |
| 1:YA:1080:C:H2' | 1:YA:1081:U:C6 | 2.53 | 0.43 |
| 1:YA:2098:U:H2' | 1:YA:2099:U:O4' | 2.17 | 0.43 |
| 1:YA:2133:G:N2 | 1:YA:2157:G:H2' | 2.34 | 0.43 |
| 4:YE:150:VAL:CG1 | 4:YE:154:LYS:HG3 | 2.47 | 0.43 |
| 4:YE:34:VAL:HG12 | 4:YE:72:VAL:HG21 | 2.00 | 0.43 |
| 7:YH:9:ILE:HG12 | 7:YH:69:ARG:HD3 | 2.01 | 0.43 |
| 32:QA:56:U:H2' | 32:QA:57:G:H8 | 1.83 | 0.43 |
| 45:QN:3:ARG:HA | 45:QN:3:ARG:HD3 | 1.77 | 0.43 |
| 51:QT:101:GLY:HA2 | 51:QT:102:GLY:HA2 | 1.68 | 0.43 |
| 53:QV:64:G:H2' | 53:QV:65:C:C6 | 2.54 | 0.43 |
| 1:RA:2394:C:OP2 | 30:R8:30:ARG:HD2 | 2.18 | 0.43 |
| 1:RA:2114:A:H3' | 1:RA:2115:G:H8 | 1.83 | 0.43 |
| 1:RA:2122:U:H3 | 1:RA:2176:A:N6 | 2.15 | 0.43 |
| 1:RA:657:U:H2' | 1:RA:658:C:C6 | 2.54 | 0.43 |
| 6:RG:131:TYR:HB3 | 6:RG:159:VAL:CG1 | 2.48 | 0.43 |
| 8:RI:75:LEU:HD22 | 8:RI:105:HIS:ND1 | 2.33 | 0.43 |
| 32:XA:839:U:H3' | 32:XA:840:C:C5 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:XP:75:ARG:HG3 | 47:XP:80:PHE:HD2 | 1.84 | 0.43 |
| 55:XY:138:TYR:CD1 | 55:XY:336:LYS:HB2 | 2.53 | 0.43 |
| 1:YA:1638:C:O3' | 1:YA:2709:G:N2 | 2.51 | 0.43 |
| 1:YA:1790:C:H5'' | 1:YA:1791:A:OP1 | 2.18 | 0.43 |
| 1:YA:1810:A:H2' | 1:YA:1811:G:O4' | 2.19 | 0.43 |
| 1:YA:2184:G:N1 | 1:YA:2185:C:O2 | 2.51 | 0.43 |
| 9:YN:62:VAL:HG11 | 9:YN:66:LYS:HB2 | 2.00 | 0.43 |
| 32:QA:1493:A:H4' | 55:QY:121:GLY:N | 2.34 | 0.43 |
| 32:QA:575:G:N2 | 32:QA:881:G:H1' | 2.33 | 0.43 |
| 34:QC:18:TRP:HZ2 | 45:QN:57:ARG:HB3 | 1.83 | 0.43 |
| 39:QH:41:ARG:NH1 | 39:QH:123:GLU:OE2 | 2.48 | 0.43 |
| 38:QG:150:ALA:HA | 42:QK:59:TYR:HB3 | 2.01 | 0.43 |
| 46:QO:61:GLY:O | 46:QO:65:ARG:HG3 | 2.19 | 0.43 |
| 26:R4:59:PHE:CE1 | 50:QS:64:GLU:HA | 2.53 | 0.43 |
| 1:RA:577:G:O2' | 1:RA:1254:A:OP1 | 2.33 | 0.43 |
| 1:RA:2086:U:H2' | 1:RA:2087:G:C8 | 2.52 | 0.43 |
| 1:RA:2186:G:C2 | 1:RA:2187:G:C5 | 3.06 | 0.43 |
| 1:RA:321:G:O2' | 1:RA:340:A:N3 | 2.51 | 0.43 |
| 6:RG:55:LYS:O | 6:RG:59:GLU:HG3 | 2.18 | 0.43 |
| 11:RP:84:ASN:OD1 | 11:RP:117:GLU:HB2 | 2.19 | 0.43 |
| 12:RQ:16:ARG:HG2 | 12:RQ:18:LYS:HD3 | 2.00 | 0.43 |
| 13:RR:104:ARG:HD2 | 13:RR:107:ASP:OD1 | 2.19 | 0.43 |
| 1:RA:2319:G:H22 | 14:RS:3:ARG:CZ | 2.32 | 0.43 |
| 14:RS:66:ALA:O | 14:RS:69:VAL:HG22 | 2.19 | 0.43 |
| 16:RU:86:ALA:O | 17:RV:49:THR:HG23 | 2.18 | 0.43 |
| 32:XA:1103:C:OP1 | 33:XB:96:ARG:NH1 | 2.50 | 0.43 |
| 32:XA:1402:4OC:H6 | 32:XA:1402:4OC:O5' | 2.19 | 0.43 |
| 32:XA:864:A:H2' | 32:XA:865:A:C8 | 2.54 | 0.43 |
| 34:XC:180:ALA:HB1 | 34:XC:203:PHE:CE1 | 2.53 | 0.43 |
| 22:Y0:50:ASN:HB3 | 22:Y0:63:VAL:HG22 | 2.00 | 0.43 |
| 1:YA:1073:A:O2' | 1:YA:1074:G:O5' | 2.36 | 0.43 |
| 1:YA:1404:C:H2' | 1:YA:1405:U:H6 | 1.83 | 0.43 |
| 1:YA:1518:U:H2' | 1:YA:1519:G:O4' | 2.19 | 0.43 |
| 1:YA:2734:A:H2' | 1:YA:2735:G:O4' | 2.18 | 0.43 |
| 1:YA:873:G:H1 | 1:YA:904:C:H42 | 1.64 | 0.43 |
| 4:YE:59:VAL:HG12 | 4:YE:64:LYS:HG3 | 2.00 | 0.43 |
| 1:YA:911:A:H2' | 12:YQ:9:TYR:OH | 2.18 | 0.43 |
| 21:YZ:23:LYS:NZ | 21:YZ:40:ASP:OD2 | 2.51 | 0.43 |
| 34:QC:36:ASP:OD1 | 34:QC:57:ILE:HG21 | 2.18 | 0.43 |
| 26:R4:50:VAL:HG13 | 44:QM:65:LYS:HG2 | 2.01 | 0.43 |
| 53:QV:4:G:O2' | 53:QV:5:G:H8 | 2.02 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:RA:1029:A:N6 | 1:RA:1125:G:O2' | 2.50 | 0.43 |
| 1:RA:184:C:H2' | 1:RA:185:U:C6 | 2.53 | 0.43 |
| 1:RA:607:U:OP1 | 5:RF:102:PRO:HA | 2.18 | 0.43 |
| 12:RQ:55:VAL:HG12 | 12:RQ:64:ILE:HD12 | 1.99 | 0.43 |
| 32:XA:1062:U:H2' | 32:XA:1063:C:C6 | 2.53 | 0.43 |
| 32:XA:114:U:H2' | 32:XA:115:G:C8 | 2.54 | 0.43 |
| 38:XG:50:ILE:HD11 | 38:XG:58:PRO:HA | 2.00 | 0.43 |
| 41:XJ:45:ARG:HG2 | 41:XJ:47:PHE:CZ | 2.54 | 0.43 |
| 32:XA:750:G:N3 | 46:XO:23:GLY:HA3 | 2.33 | 0.43 |
| 55:XY:229:SER:OG | 55:XY:242:SER:O | 2.37 | 0.43 |
| 1:YA:2526:G:C2' | 31:Y9:1:MET:H1 | 2.28 | 0.43 |
| 1:YA:2693:A:H2' | 1:YA:2694:G:C8 | 2.54 | 0.43 |
| 1:YA:370:G:H4' | 1:YA:371:A:OP2 | 2.18 | 0.43 |
| 1:YA:78:A:H2' | 1:YA:79:G:H8 | 1.83 | 0.43 |
| 5:YF:34:TRP:CH2 | 11:YP:8:PRO:HB3 | 2.54 | 0.43 |
| 6:YG:126:ASP:HB3 | 6:YG:128:ARG:H | 1.84 | 0.43 |
| 6:YG:47:LYS:HG2 | 6:YG:48:GLU:N | 2.34 | 0.43 |
| 9:YN:58:ASP:N | 9:YN:58:ASP:OD1 | 2.49 | 0.43 |
| 16:YU:49:HIS:HA | 16:YU:52:ARG:HB3 | 1.98 | 0.43 |
| 18:YW:19:LEU:HD23 | 27:Y5:25:LEU:HD21 | 2.00 | 0.43 |
| 32:QA:620:C:H2' | 32:QA:621:A:O4' | 2.19 | 0.43 |
| 42:QK:18:ARG:NH2 | 42:QK:35:PRO:O | 2.52 | 0.43 |
| 53:QV:28:C:H2' | 53:QV:29:G:H8 | 1.82 | 0.43 |
| 1:RA:1778:U:H2' | 1:RA:1784:A:N6 | 2.33 | 0.43 |
| 1:RA:2106:G:C4 | 1:RA:2107:C:H1' | 2.54 | 0.43 |
| 3:RD:145:VAL:HB | 3:RD:155:LEU:HB2 | 2.01 | 0.43 |
| 1:RA:601:C:OP1 | 5:RF:108:LYS:HE3 | 2.18 | 0.43 |
| 6:RG:106:LEU:HA | 6:RG:110:ALA:HB3 | 1.99 | 0.43 |
| 1:RA:1188:U:C4' | 17:RV:79:VAL:HG22 | 2.49 | 0.43 |
| 32:XA:537:G:H5'' | 43:XL:113:ARG:NH1 | 2.34 | 0.43 |
| 32:XA:737:A:H2' | 32:XA:738:C:H6 | 1.84 | 0.43 |
| 34:XC:148:GLY:HA3 | 34:XC:172:ARG:O | 2.19 | 0.43 |
| 35:XD:153:ARG:HG2 | 35:XD:153:ARG:H | 1.65 | 0.43 |
| 41:XJ:49:VAL:HG22 | 41:XJ:50:ILE:O | 2.18 | 0.43 |
| 43:XL:32:PHE:CD2 | 43:XL:86:ARG:HB3 | 2.54 | 0.43 |
| 44:XM:15:VAL:O | 44:XM:19:LEU:HD13 | 2.17 | 0.43 |
| 32:XA:273:A:H1' | 48:XQ:16:GLN:NE2 | 2.33 | 0.43 |
| 55:XY:328:ARG:O | 55:XY:329:LEU:HG | 2.18 | 0.43 |
| 30:Y8:63:PRO:HG2 | 30:Y8:64:TYR:CD2 | 2.54 | 0.43 |
| 1:YA:1045:A:H8 | 1:YA:1047:G:N3 | 2.17 | 0.43 |
| 1:YA:1091:G:H2' | 1:YA:1091:G:N3 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:1359:A:N6 | 1:YA:1372:U:H3 | 2.15 | 0.43 |
| 1:YA:2119:A:O2' | 1:YA:2120:G:H5' | 2.18 | 0.43 |
| 1:YA:2348:U:O4 | 1:YA:2382:G:N1 | 2.52 | 0.43 |
| 1:YA:528:A:O2' | 1:YA:529:A:H5' | 2.19 | 0.43 |
| 3:YD:142:VAL:HG23 | 3:YD:193:VAL:HA | 2.00 | 0.43 |
| 9:YN:131:GLN:CD | 9:YN:131:GLN:H | 2.21 | 0.43 |
| 1:YA:1287:A:H8 | 13:YR:104:ARG:HD3 | 1.83 | 0.43 |
| 15:YT:118:ARG:HH22 | 15:YT:121:ILE:HG21 | 1.84 | 0.43 |
| 32:QA:1323:G:H2' | 32:QA:1324:A:C8 | 2.53 | 0.43 |
| 32:QA:567:G:H2' | 32:QA:568:G:O4' | 2.19 | 0.43 |
| 33:QB:124:SER:HA | 33:QB:125:PRO:HA | 1.71 | 0.43 |
| 37:QF:89:MET:HE1 | 49:QR:72:ARG:HB3 | 2.01 | 0.43 |
| 1:RA:1179:C:H2' | 1:RA:1180:C:C6 | 2.54 | 0.43 |
| 1:RA:1530:C:N4 | 1:RA:1539:G:H1 | 2.16 | 0.43 |
| 1:RA:2389:G:H5'' | 1:RA:2390:U:O4' | 2.19 | 0.43 |
| 1:RA:251:A:C5 | 1:RA:252:G:H1' | 2.54 | 0.43 |
| 6:RG:114:ILE:HG12 | 6:RG:140:ILE:HG12 | 2.01 | 0.43 |
| 19:RX:41:ASN:O | 19:RX:45:THR:HG23 | 2.18 | 0.43 |
| 20:RY:19:LYS:HE2 | 20:RY:19:LYS:HB3 | 1.86 | 0.43 |
| 33:XB:19:HIS:CG | 33:XB:20:GLU:H | 2.36 | 0.43 |
| 34:XC:180:ALA:HB1 | 34:XC:203:PHE:HE1 | 1.84 | 0.43 |
| 39:XH:73:ASP:OD1 | 39:XH:75:ARG:HD3 | 2.19 | 0.43 |
| 45:XN:4:LYS:O | 45:XN:7:ILE:HG12 | 2.19 | 0.43 |
| 50:XS:30:LEU:HD11 | 50:XS:50:ALA:HB2 | 2.00 | 0.43 |
| 55:XY:103:LYS:HE2 | 55:XY:103:LYS:HB3 | 1.88 | 0.43 |
| 55:XY:165:LYS:HE2 | 55:XY:167:SER:OG | 2.19 | 0.43 |
| 1:YA:1058:G:N2 | 1:YA:1080:C:N3 | 2.59 | 0.43 |
| 1:YA:1530:C:HO2' | 1:YA:1531:C:P | 2.38 | 0.43 |
| 1:YA:2119:A:N6 | 1:YA:2168:G:H21 | 2.16 | 0.43 |
| 1:YA:2137:C:H1' | 1:YA:2154:G:H22 | 1.84 | 0.43 |
| 1:YA:336:C:O2' | 20:YY:35:TYR:OH | 2.34 | 0.43 |
| 1:YA:956:G:OP2 | 12:YQ:14:ARG:NH2 | 2.49 | 0.43 |
| 19:YX:56:THR:HB | 19:YX:77:LYS:HE3 | 2.01 | 0.43 |
| 20:YY:87:LYS:HB3 | 20:YY:95:LYS:HD3 | 2.00 | 0.43 |
| 32:QA:46:G:H2' | 32:QA:366:C:C5 | 2.54 | 0.43 |
| 36:QE:33:VAL:HG13 | 36:QE:112:LEU:HD12 | 2.01 | 0.43 |
| 55:QY:114:GLU:HB3 | 55:QY:163:ILE:HB | 2.01 | 0.43 |
| 1:RA:2870:C:H2' | 1:RA:2871:C:O4' | 2.19 | 0.43 |
| 1:RA:492:A:H2' | 1:RA:493:G:O4' | 2.19 | 0.43 |
| 1:RA:1971:A:P | 3:RD:242:ARG:HH22 | 2.41 | 0.43 |
| 12:RQ:110:THR:HG23 | 12:RQ:113:GLN:OE1 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:RT:60:THR:HG22 | 15:RT:77:PRO:HA | 2.01 | 0.43 |
| 32:XA:1023:G:H3' | 32:XA:1024:G:C8 | 2.50 | 0.43 |
| 32:XA:1039:C:C4 | 32:XA:1040:U:C4 | 3.06 | 0.43 |
| 32:XA:1342:C:H2' | 32:XA:1343:G:C8 | 2.54 | 0.43 |
| 1:YA:1050:A:C2 | 1:YA:1051:G:C5 | 3.06 | 0.43 |
| 1:YA:1759:A:H1' | 1:YA:2711:A:C2 | 2.54 | 0.43 |
| 7:YH:84:SER:HA | 7:YH:133:VAL:O | 2.18 | 0.43 |
| 9:YN:34:LEU:HD23 | 9:YN:107:LEU:HD11 | 2.01 | 0.43 |
| 9:YN:108:PRO:O | 9:YN:113:GLY:HA3 | 2.19 | 0.43 |
| 32:QA:1065:U:H4' | 32:QA:1066:C:O5' | 2.19 | 0.42 |
| 32:QA:320:C:O2' | 32:QA:1435:G:O2' | 2.31 | 0.42 |
| 42:QK:20:TYR:HB2 | 42:QK:31:THR:HG23 | 2.01 | 0.42 |
| 44:QM:11:ARG:C | 44:QM:13:LYS:H | 2.23 | 0.42 |
| 32:QA:1047:G:H5'' | 45:QN:4:LYS:HD3 | 2.01 | 0.42 |
| 55:QY:119:THR:HG21 | 55:QY:303:ARG:HH11 | 1.83 | 0.42 |
| 26:R4:56:VAL:HB | 26:R4:60:GLN:HG2 | 2.01 | 0.42 |
| 1:RA:1503:U:H2' | 1:RA:1504:C:C6 | 2.54 | 0.42 |
| 1:RA:2355:C:H1' | 22:R0:39:ARG:HH21 | 1.83 | 0.42 |
| 1:RA:476:G:H4' | 1:RA:502:A:N1 | 2.34 | 0.42 |
| 1:RA:886:C:O2' | 1:RA:889:C:N4 | 2.51 | 0.42 |
| 3:RD:206:LEU:HD22 | 3:RD:211:ARG:HG2 | 2.00 | 0.42 |
| 32:XA:1315:U:H2' | 32:XA:1316:G:O4' | 2.18 | 0.42 |
| 32:XA:779:C:H2' | 32:XA:780:A:O4' | 2.19 | 0.42 |
| 34:XC:164:ARG:HG2 | 34:XC:165:THR:H | 1.83 | 0.42 |
| 34:XC:77:ILE:O | 34:XC:84:ILE:N | 2.47 | 0.42 |
| 34:XC:6:HIS:NE2 | 34:XC:8:ILE:HB | 2.34 | 0.42 |
| 32:XA:1151:A:O4' | 41:XJ:39:PRO:HB2 | 2.19 | 0.42 |
| 41:XJ:70:ARG:HD3 | 41:XJ:70:ARG:HA | 1.88 | 0.42 |
| 1:YA:577:G:O2' | 1:YA:1254:A:OP1 | 2.33 | 0.42 |
| 1:YA:1798:U:H5' | 3:YD:259:THR:CG2 | 2.46 | 0.42 |
| 1:YA:2262:U:H4' | 1:YA:2328:A:H2 | 1.83 | 0.42 |
| 1:YA:78:A:H2' | 1:YA:79:G:C8 | 2.53 | 0.42 |
| 7:YH:72:ILE:O | 7:YH:75:ALA:HB3 | 2.19 | 0.42 |
| 12:YQ:11:LYS:HE2 | 12:YQ:88:GLY:O | 2.19 | 0.42 |
| 21:YZ:33:LEU:HD11 | 21:YZ:90:VAL:HG21 | 2.00 | 0.42 |
| 32:QA:159:G:H2' | 32:QA:161:A:OP2 | 2.18 | 0.42 |
| 32:QA:576:G:N2 | 32:QA:760:G:OP1 | 2.52 | 0.42 |
| 36:QE:50:GLU:HB2 | 36:QE:53:LEU:HD13 | 2.01 | 0.42 |
| 42:QK:70:LYS:HB2 | 42:QK:70:LYS:HE2 | 1.86 | 0.42 |
| 47:QP:74:LEU:O | 47:QP:79:VAL:HG22 | 2.19 | 0.42 |
| 53:QV:47:U:H3' | 53:QV:48:C:C5' | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:R3:8:LEU:CD1 | 25:R3:31:LEU:HD22 | 2.49 | 0.42 |
| 1:RA:1053:C:O2' | 1:RA:1054:A:O5' | 2.37 | 0.42 |
| 1:RA:1091:G:H2' | 1:RA:1091:G:N3 | 2.34 | 0.42 |
| 1:RA:1056:G:N1 | 1:RA:1102:C:OP2 | 2.45 | 0.42 |
| 1:RA:2051:A:H5' | 1:RA:2578:G:O4' | 2.19 | 0.42 |
| 1:RA:2390:U:O2' | 1:RA:2391:G:H5' | 2.19 | 0.42 |
| 1:RA:740:U:H2' | 1:RA:741:G:C8 | 2.54 | 0.42 |
| 6:RG:170:ARG:O | 6:RG:170:ARG:HD3 | 2.19 | 0.42 |
| 7:RH:86:GLU:HB3 | 7:RH:165:ALA:HB2 | 2.01 | 0.42 |
| 21:RZ:70:LEU:HG | 21:RZ:91:LEU:HD21 | 2.01 | 0.42 |
| 32:XA:954:G:H21 | 32:XA:1227:A:H62 | 1.67 | 0.42 |
| 32:XA:1504:G:OP1 | 32:XA:1507:A:H4' | 2.19 | 0.42 |
| 32:XA:65:U:H1' | 32:XA:66:G:OP2 | 2.18 | 0.42 |
| 33:XB:71:VAL:HG12 | 33:XB:93:VAL:CG2 | 2.49 | 0.42 |
| 43:XL:117:ARG:HB3 | 43:XL:122:THR:O | 2.19 | 0.42 |
| 55:XY:312:PHE:H | 55:XY:313:PRO:HD2 | 1.83 | 0.42 |
| 25:Y3:24:LYS:HE2 | 25:Y3:24:LYS:HB2 | 1.89 | 0.42 |
| 6:YG:101:ILE:HD13 | 26:Y4:25:TYR:HB2 | 2.01 | 0.42 |
| 1:YA:2742:C:P | 31:Y9:35:ARG:HH11 | 2.41 | 0.42 |
| 1:YA:1371:G:O2' | 1:YA:1372:U:H5 | 2.02 | 0.42 |
| 1:YA:634:C:H2' | 1:YA:635:C:C6 | 2.54 | 0.42 |
| 3:YD:38:LYS:HD2 | 3:YD:38:LYS:HA | 1.82 | 0.42 |
| 6:YG:170:ARG:NH2 | 6:YG:182:LYS:O | 2.51 | 0.42 |
| 6:YG:16:ARG:O | 6:YG:20:ILE:HG13 | 2.19 | 0.42 |
| 12:YQ:60:ARG:NH2 | 21:YZ:181:GLU:OE1 | 2.49 | 0.42 |
| 32:QA:1084:G:C5 | 32:QA:1085:U:C4 | 3.08 | 0.42 |
| 37:QF:61:LEU:HD23 | 37:QF:63:TYR:OH | 2.19 | 0.42 |
| 41:QJ:38:ILE:CG1 | 41:QJ:71:LEU:HB3 | 2.49 | 0.42 |
| 32:QA:790:A:H1' | 53:QV:38:A:H4' | 2.00 | 0.42 |
| 26:R4:59:PHE:CE1 | 50:QS:64:GLU:HG3 | 2.53 | 0.42 |
| 1:RA:1035:U:OP2 | 7:RH:59:ARG:NH2 | 2.52 | 0.42 |
| 8:RI:109:ILE:HA | 8:RI:109:ILE:HD12 | 1.76 | 0.42 |
| 16:RU:49:HIS:HA | 16:RU:52:ARG:HB3 | 2.01 | 0.42 |
| 19:RX:5:TYR:HD1 | 24:R2:33:MET:SD | 2.42 | 0.42 |
| 32:XA:18:C:H4' | 32:XA:1078:U:O2 | 2.19 | 0.42 |
| 33:XB:213:LEU:O | 33:XB:217:ARG:HB2 | 2.20 | 0.42 |
| 40:XI:37:PHE:HB3 | 40:XI:43:ALA:CB | 2.50 | 0.42 |
| 47:XP:21:VAL:HG11 | 47:XP:59:TRP:NE1 | 2.34 | 0.42 |
| 55:XY:309:THR:HG23 | 55:XY:320:HIS:NE2 | 2.34 | 0.42 |
| 23:Y1:85:LEU:HD23 | 23:Y1:89:GLU:HB3 | 2.01 | 0.42 |
| 1:YA:1153:C:H2' | 1:YA:1154:G:O4' | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:234:C:H2' | 1:YA:235:U:C6 | 2.54 | 0.42 |
| 1:YA:9:U:H3 | 1:YA:2629:A:H2 | 1.66 | 0.42 |
| 7:YH:9:ILE:HG12 | 7:YH:69:ARG:CD | 2.50 | 0.42 |
| 19:YX:44:GLU:HG3 | 19:YX:51:VAL:HG23 | 2.01 | 0.42 |
| 20:YY:7:VAL:CG1 | 20:YY:27:VAL:HG21 | 2.49 | 0.42 |
| 32:QA:437:U:H5' | 35:QD:155:LEU:HD21 | 2.01 | 0.42 |
| 32:QA:575:G:C5 | 32:QA:881:G:C2 | 3.07 | 0.42 |
| 37:QF:35:ALA:HA | 37:QF:67:MET:HB3 | 2.01 | 0.42 |
| 32:QA:553:A:H5'' | 43:QL:24:VAL:HG21 | 2.01 | 0.42 |
| 44:QM:108:ARG:NH1 | 44:QM:112:GLY:O | 2.48 | 0.42 |
| 55:QY:312:PHE:N | 55:QY:313:PRO:HD2 | 2.35 | 0.42 |
| 1:RA:1400:G:H2' | 1:RA:1401:G:C8 | 2.54 | 0.42 |
| 1:RA:2119:A:H61 | 1:RA:2168:G:H21 | 1.66 | 0.42 |
| 2:RB:90:A:N7 | 2:RB:91:C:H1' | 2.34 | 0.42 |
| 12:RQ:35:VAL:CG1 | 12:RQ:130:LYS:HB3 | 2.49 | 0.42 |
| 32:XA:528:C:H5' | 32:XA:529:G:OP2 | 2.19 | 0.42 |
| 32:XA:993:G:O6 | 32:XA:1045:C:N4 | 2.48 | 0.42 |
| 34:XC:64:VAL:O | 34:XC:99:VAL:HA | 2.19 | 0.42 |
| 39:XH:98:LYS:HE3 | 39:XH:98:LYS:HB2 | 1.80 | 0.42 |
| 41:XJ:21:GLN:O | 41:XJ:25:GLU:HG2 | 2.20 | 0.42 |
| 47:XP:66:PRO:HG2 | 47:XP:71:ARG:NH1 | 2.34 | 0.42 |
| 1:YA:1036:G:H1 | 1:YA:1119:C:H42 | 1.67 | 0.42 |
| 1:YA:1493:C:C5 | 1:YA:2206:G:H2' | 2.54 | 0.42 |
| 1:YA:2144:U:H1' | 1:YA:2147:G:O6 | 2.19 | 0.42 |
| 1:YA:2693:A:H2' | 1:YA:2694:G:H8 | 1.84 | 0.42 |
| 6:YG:9:ARG:NH1 | 6:YG:13:GLU:OE1 | 2.45 | 0.42 |
| 8:YI:48:GLU:HG3 | 8:YI:52:ARG:HH11 | 1.83 | 0.42 |
| 15:YT:28:VAL:HG13 | 15:YT:86:ILE:HG23 | 2.00 | 0.42 |
| 32:QA:1518:MA6:H93 | 32:QA:1519:MA6:H92 | 2.02 | 0.42 |
| 36:QE:57:LYS:HG2 | 36:QE:61:TYR:HE2 | 1.81 | 0.42 |
| 37:QF:23:LYS:NZ | 37:QF:42:GLU:OE2 | 2.29 | 0.42 |
| 32:QA:1125:U:H4' | 41:QJ:5:ARG:NH2 | 2.34 | 0.42 |
| 55:QY:184:VAL:O | 55:QY:198:THR:HA | 2.18 | 0.42 |
| 1:RA:1668:A:O2' | 1:RA:1674:G:N7 | 2.48 | 0.42 |
| 1:RA:2320:A:N3 | 1:RA:2320:A:H2' | 2.34 | 0.42 |
| 1:RA:493:G:H2' | 1:RA:494:G:O4' | 2.19 | 0.42 |
| 1:RA:828:U:H4' | 1:RA:831:G:N1 | 2.34 | 0.42 |
| 3:RD:242:ARG:HD3 | 3:RD:242:ARG:N | 2.34 | 0.42 |
| 11:RP:101:VAL:HA | 11:RP:106:LEU:O | 2.19 | 0.42 |
| 12:RQ:35:VAL:HG13 | 12:RQ:130:LYS:HB3 | 2.01 | 0.42 |
| 20:RY:20:TYR:O | 20:RY:23:ARG:HB2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 32:XA:1004:A:H5' | 32:XA:1025:U:C5 | 2.48 | 0.42 |
| 32:XA:1402:4OC:HM41 | 54:XX:18:G:OP2 | 2.18 | 0.42 |
| 40:XI:112:LYS:HE2 | 40:XI:117:HIS:O | 2.19 | 0.42 |
| 32:XA:101:A:H5' | 51:XT:10:LEU:HD21 | 2.02 | 0.42 |
| 1:YA:125:G:N3 | 29:Y7:48:LYS:HE2 | 2.34 | 0.42 |
| 1:YA:1019:U:H2' | 1:YA:1020:A:C8 | 2.54 | 0.42 |
| 1:YA:2321:G:HO2' | 1:YA:2322:A:P | 2.40 | 0.42 |
| 1:YA:2390:U:O2' | 1:YA:2391:G:H5' | 2.20 | 0.42 |
| 1:YA:2757:A:N3 | 7:YH:63:SER:OG | 2.52 | 0.42 |
| 1:YA:861:A:H2' | 1:YA:862:G:O4' | 2.19 | 0.42 |
| 1:YA:945:A:C4 | 1:YA:2448:A:C2 | 3.07 | 0.42 |
| 32:QA:1024:G:N3 | 32:QA:1024:G:H2' | 2.34 | 0.42 |
| 35:QD:8:VAL:HG22 | 35:QD:21:LEU:HD13 | 2.01 | 0.42 |
| 38:QG:113:GLU:HG3 | 38:QG:118:VAL:HG12 | 2.00 | 0.42 |
| 44:QM:74:VAL:O | 44:QM:78:ILE:HG13 | 2.20 | 0.42 |
| 55:QY:325:THR:O | 55:QY:325:THR:OG1 | 2.34 | 0.42 |
| 26:R4:57:GLU:CB | 26:R4:58:ARG:HA | 2.48 | 0.42 |
| 1:RA:1291:C:H2' | 1:RA:1292:U:C6 | 2.55 | 0.42 |
| 1:RA:1288:U:C2 | 1:RA:1327:C:O2 | 2.73 | 0.42 |
| 1:RA:1430:C:H2' | 1:RA:1431:U:C6 | 2.55 | 0.42 |
| 1:RA:1504:C:H2' | 1:RA:1505:C:C6 | 2.54 | 0.42 |
| 1:RA:330:A:HO2' | 1:RA:331:A:H8 | 1.62 | 0.42 |
| 2:RB:14:U:O3' | 2:RB:108:U:O2' | 2.37 | 0.42 |
| 4:RE:116:VAL:HG13 | 4:RE:122:PHE:HB2 | 2.01 | 0.42 |
| 21:RZ:140:ASP:OD1 | 21:RZ:142:SER:OG | 2.38 | 0.42 |
| 32:XA:1030(B):G:H21 | 32:XA:1030(D):G:H3' | 1.84 | 0.42 |
| 32:XA:1301:U:O2' | 32:XA:1302:U:H5' | 2.19 | 0.42 |
| 32:XA:796:C:O5' | 32:XA:796:C:H6 | 2.03 | 0.42 |
| 33:XB:118:LEU:HD23 | 33:XB:118:LEU:HA | 1.87 | 0.42 |
| 33:XB:58:ILE:CG2 | 33:XB:222:ILE:HG22 | 2.50 | 0.42 |
| 33:XB:178:ARG:NH2 | 39:XH:74:PRO:HB3 | 2.35 | 0.42 |
| 39:XH:82:HIS:NE2 | 39:XH:84:ARG:HG2 | 2.35 | 0.42 |
| 46:XO:35:ARG:HH21 | 46:XO:59:MET:HE2 | 1.84 | 0.42 |
| 47:XP:4:ILE:HG23 | 47:XP:36:ILE:HD11 | 2.01 | 0.42 |
| 50:XS:20:LEU:HA | 50:XS:23:ASN:HB2 | 2.02 | 0.42 |
| 55:XY:322:ILE:HD12 | 55:XY:324:LEU:HD13 | 2.02 | 0.42 |
| 1:YA:1065:U:H4' | 1:YA:1066:U:C5' | 2.48 | 0.42 |
| 1:YA:1092:C:O2 | 1:YA:1092:C:H2' | 2.18 | 0.42 |
| 1:YA:1108:U:H3' | 1:YA:1109:C:C6 | 2.54 | 0.42 |
| 1:YA:1139:G:O2' | 1:YA:1143:A:N1 | 2.43 | 0.42 |
| 1:YA:1529:G:C6 | 1:YA:1530:C:N4 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:YA:1668:A:H4' | 1:YA:1669:A:O5' | 2.18 | 0.42 |
| 1:YA:1695:G:H1' | 3:YD:8:PRO:O | 2.20 | 0.42 |
| 1:YA:2109:U:H2' | 1:YA:2110:G:C8 | 2.54 | 0.42 |
| 5:YF:135:LYS:HG3 | 5:YF:137:LYS:HG2 | 2.01 | 0.42 |
| 7:YH:154:PRO:HB3 | 7:YH:163:TYR:CE2 | 2.54 | 0.42 |
| 10:YO:26:LYS:O | 10:YO:30:ALA:HB2 | 2.20 | 0.42 |
| 21:YZ:140:ASP:OD1 | 21:YZ:142:SER:OG | 2.38 | 0.42 |
| 32:QA:1504:G:OP1 | 32:QA:1507:A:H4' | 2.20 | 0.42 |
| 35:QD:188:LEU:HA | 35:QD:189:PRO:HD3 | 1.90 | 0.42 |
| 35:QD:173:TRP:CG | 35:QD:189:PRO:HG3 | 2.54 | 0.42 |
| 40:QI:46:ALA:HB2 | 40:QI:74:ILE:HG23 | 2.02 | 0.42 |
| 41:QJ:30:SER:OG | 41:QJ:81:THR:HG22 | 2.18 | 0.42 |
| 32:QA:1302:U:C5 | 44:QM:17:VAL:HG21 | 2.55 | 0.42 |
| 45:QN:45:ARG:O | 45:QN:49:HIS:HD2 | 2.01 | 0.42 |
| 1:RA:1057:A:N6 | 1:RA:1087:G:OP2 | 2.53 | 0.42 |
| 1:RA:1069:A:H5' | 1:RA:1096:A:H5' | 2.02 | 0.42 |
| 1:RA:1092:C:O2 | 1:RA:1092:C:H2' | 2.18 | 0.42 |
| 1:RA:1022:G:C5 | 1:RA:1140:C:C4 | 3.08 | 0.42 |
| 1:RA:1418:G:H8 | 1:RA:1418:G:O5' | 2.02 | 0.42 |
| 1:RA:1570:A:H2' | 1:RA:1571:A:C8 | 2.54 | 0.42 |
| 1:RA:641:C:O2' | 1:RA:2350:C:OP1 | 2.31 | 0.42 |
| 1:RA:250:G:C6 | 1:RA:251:A:C6 | 3.08 | 0.42 |
| 1:RA:582:G:H2' | 1:RA:583:G:C8 | 2.54 | 0.42 |
| 8:RI:72:LEU:HD12 | 8:RI:138:ILE:HG21 | 2.01 | 0.42 |
| 15:RT:105:LEU:HA | 15:RT:105:LEU:HD23 | 1.89 | 0.42 |
| 37:XF:10:LEU:HB2 | 37:XF:59:TYR:HB3 | 2.01 | 0.42 |
| 26:Y4:61:ARG:HD3 | 50:XS:67:VAL:HG12 | 2.02 | 0.42 |
| 51:XT:37:SER:O | 51:XT:41:ILE:HG12 | 2.20 | 0.42 |
| 1:YA:1055:G:H2' | 1:YA:1056:G:O4' | 2.19 | 0.42 |
| 1:YA:1504:C:H2' | 1:YA:1505:C:C6 | 2.54 | 0.42 |
| 1:YA:1641:A:H2' | 1:YA:1642:G:O4' | 2.19 | 0.42 |
| 1:YA:2112:G:H2' | 1:YA:2113:U:C6 | 2.55 | 0.42 |
| 1:YA:724:U:H2' | 1:YA:725:G:O4' | 2.20 | 0.42 |
| 1:YA:875:G:H2' | 1:YA:876:C:O4' | 2.20 | 0.42 |
| 2:YB:78:A:C2 | 2:YB:100:A:C4 | 3.08 | 0.42 |
| 5:YF:129:PHE:O | 5:YF:132:VAL:HG22 | 2.19 | 0.42 |
| 32:QA:571:U:H2' | 32:QA:917:G:H4' | 2.01 | 0.42 |
| 33:QB:51:LEU:HD23 | 33:QB:201:ILE:HD12 | 2.02 | 0.42 |
| 32:QA:1232:U:H5" | 40:QI:124:GLN:O | 2.20 | 0.42 |
| 45:QN:32:SER:HB3 | 45:QN:41:ARG:HG2 | 2.01 | 0.42 |
| 45:QN:4:LYS:HG3 | 45:QN:7:ILE:HD11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:QP:79:VAL:HG23 | 47:QP:80:PHE:CD1 | 2.54 | 0.42 |
| 51:QT:92:LEU:O | 51:QT:96:GLY:N | 2.48 | 0.42 |
| 1:RA:1668:A:H4' | 1:RA:1669:A:O5' | 2.20 | 0.42 |
| 1:RA:196:A:H2' | 1:RA:196:A:N3 | 2.35 | 0.42 |
| 1:RA:2119:A:N6 | 1:RA:2168:G:H21 | 2.16 | 0.42 |
| 1:RA:2118:U:H5 | 1:RA:2148:G:H1' | 1.85 | 0.42 |
| 1:RA:2321:G:HO2' | 1:RA:2322:A:P | 2.42 | 0.42 |
| 1:RA:898:C:H2' | 1:RA:899:A:O4' | 2.20 | 0.42 |
| 2:RB:8:U:O3' | 14:RS:25:ARG:NH2 | 2.38 | 0.42 |
| 3:RD:77:ALA:HB2 | 3:RD:97:TYR:CD2 | 2.55 | 0.42 |
| 10:RO:2:ILE:HD12 | 10:RO:6:THR:HG21 | 2.01 | 0.42 |
| 32:XA:1318:A:O2' | 50:XS:37:ARG:HD2 | 2.19 | 0.42 |
| 51:XT:72:LEU:HD23 | 51:XT:72:LEU:HA | 1.89 | 0.42 |
| 55:XY:341:ILE:O | 55:XY:345:ILE:HG13 | 2.20 | 0.42 |
| 24:Y2:38:GLN:HB3 | 24:Y2:44:LEU:HB2 | 2.01 | 0.42 |
| 1:YA:760:G:H2' | 1:YA:761:A:O4' | 2.20 | 0.42 |
| 2:YB:78:A:H2' | 2:YB:79:C:O4' | 2.19 | 0.42 |
| 5:YF:129:PHE:CD2 | 5:YF:163:VAL:HG21 | 2.54 | 0.42 |
| 32:QA:1187:G:H4' | 40:QI:111:ARG:NH1 | 2.35 | 0.42 |
| 32:QA:604:G:C6 | 32:QA:635:G:C6 | 3.08 | 0.42 |
| 1:RA:1045:A:N3 | 1:RA:1045:A:H2' | 2.35 | 0.42 |
| 1:RA:1110:G:H1' | 1:RA:1111:A:C8 | 2.54 | 0.42 |
| 1:RA:1292:U:H2' | 1:RA:1293:C:C6 | 2.55 | 0.42 |
| 1:RA:1300:U:C2 | 1:RA:1626:G:C6 | 3.08 | 0.42 |
| 1:RA:276:A:H5'' | 1:RA:277:C:H5' | 2.01 | 0.42 |
| 1:RA:334:C:OP1 | 1:RA:335:C:N4 | 2.53 | 0.42 |
| 1:RA:569:U:C4 | 1:RA:570:G:C6 | 3.08 | 0.42 |
| 1:RA:581:C:H2' | 1:RA:582:G:C8 | 2.55 | 0.42 |
| 1:RA:612:C:H2' | 1:RA:613:G:O4' | 2.20 | 0.42 |
| 4:RE:101:ARG:CZ | 4:RE:171:GLU:HB2 | 2.50 | 0.42 |
| 6:RG:66:GLN:HB3 | 6:RG:92:VAL:HG21 | 2.02 | 0.42 |
| 32:XA:1005:A:C5 | 32:XA:1006:C:H1' | 2.55 | 0.42 |
| 32:XA:110:C:H2' | 32:XA:111:G:O4' | 2.19 | 0.42 |
| 32:XA:343:U:O3' | 32:XA:344:A:H8 | 2.03 | 0.42 |
| 32:XA:688:G:H2' | 32:XA:689:C:H6 | 1.84 | 0.42 |
| 34:XC:54:ARG:NH1 | 34:XC:54:ARG:HB3 | 2.35 | 0.42 |
| 41:XJ:19:SER:O | 41:XJ:23:ILE:HG12 | 2.19 | 0.42 |
| 47:XP:17:TYR:HE1 | 47:XP:41:PRO:HG3 | 1.84 | 0.42 |
| 51:XT:43:LEU:HD13 | 51:XT:51:GLU:HB3 | 2.00 | 0.42 |
| 52:XU:12:LYS:HB3 | 52:XU:22:ARG:HD2 | 2.01 | 0.42 |
| 53:XV:3:C:C2' | 53:XV:4:G:H5' | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 55:XY:123:GLU:HG3 | 55:XY:188:PRO:HB3 | 2.02 | 0.42 |
| 55:XY:333:MET:HG2 | 55:XY:333:MET:H | 1.50 | 0.42 |
| 1:YA:468:G:N7 | 29:Y7:39:ARG:NH2 | 2.59 | 0.42 |
| 1:YA:1826:G:H4' | 3:YD:242:ARG:NH1 | 2.35 | 0.42 |
| 12:YQ:32:TYR:OH | 12:YQ:111:GLU:OE1 | 2.29 | 0.42 |
| 32:QA:1023:G:H2' | 32:QA:1024:G:N7 | 2.35 | 0.42 |
| 35:QD:61:LYS:HD2 | 35:QD:207:TYR:OH | 2.20 | 0.42 |
| 35:QD:57:ARG:HH22 | 36:QE:107:ARG:HD3 | 1.85 | 0.42 |
| 55:QY:312:PHE:H | 55:QY:313:PRO:HD2 | 1.85 | 0.42 |
| 55:QY:311:ASN:ND2 | 55:QY:314:GLN:HB2 | 2.35 | 0.42 |
| 1:RA:1073:A:O2' | 1:RA:1074:G:O5' | 2.36 | 0.42 |
| 1:RA:1080:C:H2' | 1:RA:1081:U:C6 | 2.55 | 0.42 |
| 1:RA:1607:C:N4 | 1:RA:1622:G:OP2 | 2.34 | 0.42 |
| 1:RA:2282:G:OP1 | 1:RA:2283:C:H1' | 2.19 | 0.42 |
| 4:RE:150:VAL:CG1 | 4:RE:154:LYS:HG3 | 2.50 | 0.42 |
| 10:RO:26:LYS:O | 10:RO:30:ALA:HB2 | 2.19 | 0.42 |
| 32:XA:1442(A):G:N3 | 32:XA:1442(A):G:H2' | 2.34 | 0.42 |
| 32:XA:148:G:H2' | 32:XA:149:A:C8 | 2.55 | 0.42 |
| 32:XA:148:G:H2' | 32:XA:149:A:H8 | 1.85 | 0.42 |
| 32:XA:163:C:H2' | 32:XA:164:U:O4' | 2.19 | 0.42 |
| 32:XA:448:A:P | 32:XA:485:G:H22 | 2.41 | 0.42 |
| 32:XA:567:G:H2' | 32:XA:568:G:O4' | 2.20 | 0.42 |
| 32:XA:745:C:H1' | 32:XA:836:G:O2' | 2.20 | 0.42 |
| 32:XA:1151:A:H5" | 41:XJ:41:PRO:HA | 2.02 | 0.42 |
| 50:XS:23:ASN:HA | 50:XS:27:GLU:OE2 | 2.20 | 0.42 |
| 55:XY:101:LEU:H | 55:XY:102:PRO:HD2 | 1.84 | 0.42 |
| 55:XY:211:ASP:OD1 | 55:XY:286:ARG:NH2 | 2.52 | 0.42 |
| 1:YA:1022:G:C5 | 1:YA:1140:C:C4 | 3.07 | 0.42 |
| 1:YA:1179:C:H2' | 1:YA:1180:C:C6 | 2.55 | 0.42 |
| 1:YA:1510:G:H2' | 1:YA:1511:C:C6 | 2.55 | 0.42 |
| 7:YH:90:LYS:HD3 | 7:YH:159:GLU:HG2 | 2.02 | 0.42 |
| 8:YI:129:THR:HA | 8:YI:138:ILE:O | 2.20 | 0.42 |
| 32:QA:107:G:H2' | 32:QA:108:G:O4' | 2.20 | 0.41 |
| 32:QA:112:G:H4' | 32:QA:389:A:H4' | 2.02 | 0.41 |
| 33:QB:47:THR:HA | 33:QB:202:PRO:HG2 | 2.02 | 0.41 |
| 36:QE:69:VAL:HA | 36:QE:70:PRO:HD3 | 1.78 | 0.41 |
| 42:QK:79:SER:HA | 42:QK:104:GLN:HB2 | 2.01 | 0.41 |
| 44:QM:13:LYS:HA | 44:QM:44:ARG:NH1 | 2.34 | 0.41 |
| 50:QS:52:TYR:HB2 | 50:QS:57:HIS:CD2 | 2.54 | 0.41 |
| 55:QY:222:LEU:HD13 | 55:QY:246:ILE:HG21 | 2.01 | 0.41 |
| 1:RA:1057:A:C2 | 1:RA:1058:G:C4 | 3.07 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:RA:2188:C:H2' | 1:RA:2189:U:O4' | 2.20 | 0.41 |
| 1:RA:2648:C:H2' | 1:RA:2649:U:C6 | 2.55 | 0.41 |
| 1:RA:2690:C:N4 | 1:RA:2713:A:H1' | 2.35 | 0.41 |
| 32:XA:1003:G:H3' | 32:XA:1003:G:N3 | 2.35 | 0.41 |
| 32:XA:1206:G:H2' | 32:XA:1207:2MG:O4' | 2.20 | 0.41 |
| 32:XA:501:C:H2' | 32:XA:502:G:H8 | 1.83 | 0.41 |
| 32:XA:859:A:H2' | 32:XA:860:A:O4' | 2.20 | 0.41 |
| 34:XC:6:HIS:HB3 | 45:XN:49:HIS:ND1 | 2.35 | 0.41 |
| 40:X1:108:VAL:HG12 | 40:X1:109:VAL:H | 1.85 | 0.41 |
| 41:XJ:16:LEU:HD13 | 41:XJ:70:ARG:HG2 | 2.02 | 0.41 |
| 32:XA:1492:A:O4' | 43:XL:47:LYS:HD3 | 2.18 | 0.41 |
| 51:XT:42:GLN:O | 51:XT:45:GLN:HB3 | 2.20 | 0.41 |
| 1:YA:1057:A:H62 | 1:YA:1087:G:P | 2.43 | 0.41 |
| 1:YA:1068:G:H3' | 1:YA:1096:A:OP2 | 2.20 | 0.41 |
| 1:YA:1166:C:H2' | 1:YA:1167:U:C6 | 2.55 | 0.41 |
| 1:YA:1316:U:H2' | 1:YA:1317:A:C8 | 2.55 | 0.41 |
| 1:YA:1753:G:OP1 | 15:YT:95:ARG:HD3 | 2.20 | 0.41 |
| 1:YA:180:G:OP2 | 29:Y7:32:LYS:HE3 | 2.20 | 0.41 |
| 1:YA:2271:G:OP1 | 22:Y0:18:ALA:HB1 | 2.20 | 0.41 |
| 1:YA:228:A:H8 | 1:YA:229:A:H5' | 1.85 | 0.41 |
| 1:YA:30:G:H2' | 1:YA:31:C:C6 | 2.54 | 0.41 |
| 7:YH:55:PRO:HG2 | 7:YH:61:HIS:ND1 | 2.35 | 0.41 |
| 9:YN:67:LEU:HD13 | 9:YN:67:LEU:HA | 1.96 | 0.41 |
| 12:YQ:130:LYS:HB3 | 12:YQ:130:LYS:HE2 | 1.88 | 0.41 |
| 20:YY:20:TYR:CE1 | 20:YY:43:ASN:HA | 2.55 | 0.41 |
| 32:QA:1077:G:N2 | 32:QA:1080:A:OP2 | 2.52 | 0.41 |
| 32:QA:110:C:H2' | 32:QA:111:G:O4' | 2.21 | 0.41 |
| 32:QA:713:G:H2' | 32:QA:714:G:C8 | 2.55 | 0.41 |
| 34:QC:3:ASN:N | 34:QC:3:ASN:OD1 | 2.52 | 0.41 |
| 39:QH:81:HIS:N | 39:QH:138:TRP:O | 2.53 | 0.41 |
| 55:QY:219:PRO:C | 55:QY:221:ASP:H | 2.24 | 0.41 |
| 23:R1:3:LYS:HG2 | 23:R1:61:ARG:NH1 | 2.34 | 0.41 |
| 1:RA:2420:C:H5'' | 28:R6:8:LYS:CD | 2.50 | 0.41 |
| 1:RA:2461:C:H2' | 1:RA:2462:U:C6 | 2.54 | 0.41 |
| 6:RG:138:GLN:HE22 | 6:RG:153:ARG:HD2 | 1.84 | 0.41 |
| 7:RH:98:LEU:HA | 7:RH:98:LEU:HD12 | 1.93 | 0.41 |
| 32:XA:1151:A:O2' | 32:XA:1152:A:O5' | 2.34 | 0.41 |
| 32:XA:1068:G:N2 | 32:XA:1191:A:N3 | 2.61 | 0.41 |
| 32:XA:600:C:H2' | 32:XA:601:C:C6 | 2.55 | 0.41 |
| 42:XK:92:GLU:O | 42:XK:96:ARG:HG2 | 2.20 | 0.41 |
| 43:XL:117:ARG:NH2 | 43:XL:124:LYS:HB2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 32:XA:523:A:N1 | 43:XL:92:0TD:H6 | 2.35 | 0.41 |
| 46:XO:61:GLY:O | 46:XO:65:ARG:HG3 | 2.20 | 0.41 |
| 48:XQ:6:LEU:O | 48:XQ:58:GLU:HA | 2.20 | 0.41 |
| 29:Y7:12:ARG:NH2 | 29:Y7:44:PRO:HB3 | 2.36 | 0.41 |
| 1:YA:1053:C:H4' | 1:YA:1054:A:OP1 | 2.20 | 0.41 |
| 1:YA:2810:A:N6 | 1:YA:2891:G:O2' | 2.40 | 0.41 |
| 1:YA:478:A:C6 | 1:YA:480:A:C6 | 3.08 | 0.41 |
| 1:YA:748:G:OP1 | 1:YA:2612:C:N4 | 2.53 | 0.41 |
| 5:YF:53:THR:HG22 | 5:YF:56:GLU:OE2 | 2.20 | 0.41 |
| 6:YG:126:ASP:HB2 | 6:YG:130:ASN:O | 2.20 | 0.41 |
| 7:YH:163:TYR:CE2 | 7:YH:169:VAL:HG22 | 2.55 | 0.41 |
| 7:YH:98:LEU:HD12 | 7:YH:98:LEU:HA | 1.91 | 0.41 |
| 8:YI:62:LYS:HE2 | 8:YI:133:HIS:NE2 | 2.35 | 0.41 |
| 18:YW:9:TYR:HA | 18:YW:100:THR:CG2 | 2.49 | 0.41 |
| 32:QA:1007:C:N3 | 32:QA:1022:G:O6 | 2.53 | 0.41 |
| 33:QB:8:LYS:HG2 | 33:QB:8:LYS:H | 1.60 | 0.41 |
| 30:R8:33:ASN:HA | 30:R8:36:LYS:HD2 | 2.02 | 0.41 |
| 1:RA:1405:U:H2' | 1:RA:1406:U:C6 | 2.54 | 0.41 |
| 1:RA:458:G:O2' | 1:RA:469:G:O6 | 2.22 | 0.41 |
| 9:RN:58:ASP:N | 9:RN:58:ASP:OD1 | 2.52 | 0.41 |
| 1:RA:2820:A:P | 13:RR:2:ARG:HH22 | 2.43 | 0.41 |
| 32:XA:1030(B):G:H1' | 32:XA:1030(D):G:C5 | 2.55 | 0.41 |
| 32:XA:1065:U:H4' | 32:XA:1066:C:O5' | 2.20 | 0.41 |
| 32:XA:297:G:N2 | 32:XA:300:A:OP2 | 2.44 | 0.41 |
| 35:XD:189:PRO:HB2 | 35:XD:194:LEU:HD11 | 2.02 | 0.41 |
| 55:XY:195:ARG:HE | 55:XY:197:HIS:CE1 | 2.38 | 0.41 |
| 55:XY:209:LEU:HD12 | 55:XY:209:LEU:HA | 1.88 | 0.41 |
| 1:YA:1639:U:C2' | 1:YA:1640:C:H5'' | 2.49 | 0.41 |
| 1:YA:2331:G:O2' | 1:YA:2336:A:N1 | 2.45 | 0.41 |
| 1:YA:2785:C:O2' | 4:YE:66:HIS:ND1 | 2.42 | 0.41 |
| 6:YG:115:ARG:HG2 | 6:YG:136:ARG:HH21 | 1.85 | 0.41 |
| 32:QA:1298:C:H4' | 32:QA:1299:A:C4 | 2.55 | 0.41 |
| 32:QA:942:G:C2 | 32:QA:1342:C:C2 | 3.08 | 0.41 |
| 35:QD:156:GLU:O | 35:QD:160:GLN:HG2 | 2.20 | 0.41 |
| 40:QI:108:VAL:HG12 | 40:QI:109:VAL:N | 2.36 | 0.41 |
| 41:QJ:38:ILE:O | 41:QJ:38:ILE:HG13 | 2.19 | 0.41 |
| 1:RA:1270:C:H5'' | 1:RA:1271:G:O5' | 2.20 | 0.41 |
| 1:RA:1941:C:C5 | 1:RA:1942:5MC:HM52 | 2.56 | 0.41 |
| 1:RA:2695:C:H2' | 1:RA:2696:U:C6 | 2.55 | 0.41 |
| 1:RA:337:C:H2' | 1:RA:338:G:O4' | 2.20 | 0.41 |
| 1:RA:721:C:H2' | 1:RA:722:A:H8 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:RA:955:C:OP1 | 12:RQ:87:LYS:HE2 | 2.20 | 0.41 |
| 1:RA:9:U:H3 | 1:RA:2629:A:H2 | 1.65 | 0.41 |
| 5:RF:101:LEU:HD12 | 5:RF:102:PRO:HD2 | 2.01 | 0.41 |
| 5:RF:116:ASP:OD1 | 5:RF:119:ARG:NH2 | 2.48 | 0.41 |
| 7:RH:12:PRO:O | 7:RH:15:VAL:HG22 | 2.20 | 0.41 |
| 32:XA:1005:A:H5'' | 32:XA:1006:C:C6 | 2.55 | 0.41 |
| 32:XA:1070:U:H2' | 32:XA:1071:C:H6 | 1.84 | 0.41 |
| 32:XA:262:A:C6 | 32:XA:263:A:C6 | 3.07 | 0.41 |
| 32:XA:552:U:O3' | 43:XL:87:GLY:HA2 | 2.20 | 0.41 |
| 32:XA:560:U:H4' | 32:XA:561:U:O5' | 2.19 | 0.41 |
| 33:XB:127:ILE:HG12 | 33:XB:128:GLU:H | 1.85 | 0.41 |
| 47:XP:19:ILE:HG22 | 47:XP:36:ILE:HG13 | 2.01 | 0.41 |
| 53:XV:10:G:N2 | 53:XV:26:G:H1' | 2.35 | 0.41 |
| 53:XV:16:C:O2' | 53:XV:61:C:OP1 | 2.34 | 0.41 |
| 55:XY:129:GLY:O | 55:XY:133:ARG:HG2 | 2.20 | 0.41 |
| 55:XY:311:ASN:HD21 | 55:XY:313:PRO:HG2 | 1.85 | 0.41 |
| 1:YA:1030:G:N1 | 1:YA:1124:C:O2 | 2.50 | 0.41 |
| 1:YA:1449:A:N3 | 1:YA:1529:G:H1' | 2.36 | 0.41 |
| 1:YA:1709:U:H2' | 1:YA:1710:C:C6 | 2.54 | 0.41 |
| 1:YA:385:C:O2 | 11:YP:71:VAL:HG21 | 2.20 | 0.41 |
| 2:YB:33:G:C6 | 2:YB:34:U:C4 | 3.09 | 0.41 |
| 15:YT:16:ARG:HD3 | 15:YT:18:ASP:OD1 | 2.20 | 0.41 |
| 1:YA:1187:G:H5' | 17:YV:81:TYR:CE1 | 2.55 | 0.41 |
| 32:QA:141:A:H1' | 32:QA:182:U:O2 | 2.21 | 0.41 |
| 33:QB:224:GLN:HA | 33:QB:228:GLY:O | 2.21 | 0.41 |
| 38:QG:16:LEU:HD11 | 40:QI:45:ALA:HB2 | 2.02 | 0.41 |
| 23:R1:82:LEU:HA | 23:R1:82:LEU:HD23 | 1.90 | 0.41 |
| 26:R4:13:ARG:HB3 | 26:R4:15:ILE:HD11 | 2.03 | 0.41 |
| 1:RA:1063:G:H2' | 1:RA:1065:U:C6 | 2.55 | 0.41 |
| 1:RA:154(B):C:H42 | 1:RA:171:G:H1 | 1.68 | 0.41 |
| 1:RA:2680:C:OP2 | 4:RE:111:ARG:NH2 | 2.53 | 0.41 |
| 1:RA:27:G:C2 | 1:RA:512:G:N3 | 2.89 | 0.41 |
| 1:RA:370:G:H4' | 1:RA:371:A:OP2 | 2.20 | 0.41 |
| 6:RG:77:ILE:HB | 6:RG:82:LEU:HB3 | 2.02 | 0.41 |
| 1:RA:583:G:OP2 | 16:RU:10:ARG:HD2 | 2.20 | 0.41 |
| 20:RY:15:VAL:HG21 | 20:RY:42:VAL:HG11 | 2.02 | 0.41 |
| 21:RZ:91:LEU:HD12 | 21:RZ:130:PRO:HG3 | 2.03 | 0.41 |
| 32:XA:1201:A:H4' | 32:XA:1202:G:H5'' | 2.03 | 0.41 |
| 32:XA:663:A:H5' | 32:XA:836:G:OP1 | 2.21 | 0.41 |
| 36:XE:60:TYR:CZ | 36:XE:64:ARG:HD3 | 2.56 | 0.41 |
| 40:XI:42:ARG:HB3 | 40:XI:42:ARG:HE | 1.62 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:YN:50:LYS:HA | 45:YN:50:LYS:HD2 | 1.79 | 0.41 |
| 45:YN:58:LYS:HE3 | 45:YN:58:LYS:HB3 | 1.88 | 0.41 |
| 32:XA:1305:G:H5' | 52:XU:4:GLY:HA3 | 2.02 | 0.41 |
| 30:Y8:23:VAL:CG1 | 30:Y8:47:LYS:HD3 | 2.50 | 0.41 |
| 1:YA:1048:A:C5 | 1:YA:1049:C:C4 | 3.09 | 0.41 |
| 1:YA:1025:G:C4 | 1:YA:1135:C:H1' | 2.55 | 0.41 |
| 1:YA:1802:A:N1 | 1:YA:1822:G:H1' | 2.36 | 0.41 |
| 1:YA:2130:U:H2' | 1:YA:2158:A:N1 | 2.36 | 0.41 |
| 1:YA:2591:C:H2' | 1:YA:2592:G:C8 | 2.55 | 0.41 |
| 1:YA:2748:A:C2 | 1:YA:2749:A:C4 | 3.08 | 0.41 |
| 1:YA:2748:A:C6 | 1:YA:2749:A:C6 | 3.08 | 0.41 |
| 3:YD:134:ARG:NH1 | 3:YD:188:GLU:OE2 | 2.48 | 0.41 |
| 5:YF:184:TYR:CE1 | 11:YP:3:LEU:HD21 | 2.54 | 0.41 |
| 21:YZ:53:ILE:HG22 | 21:YZ:71:VAL:O | 2.21 | 0.41 |
| 34:QC:15:THR:HG21 | 34:QC:181:ASN:HA | 2.02 | 0.41 |
| 39:QH:34:GLU:OE1 | 39:QH:37:ARG:NH1 | 2.54 | 0.41 |
| 44:QM:80:ARG:O | 44:QM:84:ILE:HG23 | 2.21 | 0.41 |
| 55:QY:214:LEU:N | 55:QY:215:PRO:HD3 | 2.36 | 0.41 |
| 1:RA:1002:G:H2' | 1:RA:1003:G:O4' | 2.20 | 0.41 |
| 1:RA:1057:A:O2' | 1:RA:1058:G:P | 2.79 | 0.41 |
| 1:RA:1479:G:H1' | 1:RA:1558:A:OP1 | 2.21 | 0.41 |
| 1:RA:1810:A:H2' | 1:RA:1811:G:O4' | 2.21 | 0.41 |
| 1:RA:1827:C:OP2 | 3:RD:222:ARG:HD2 | 2.20 | 0.41 |
| 1:RA:2306:C:C4 | 1:RA:2307:G:C6 | 3.08 | 0.41 |
| 1:RA:2336:A:H61 | 22:R0:43:THR:CG2 | 2.34 | 0.41 |
| 1:RA:2342:C:O2' | 1:RA:2374:C:H5'' | 2.21 | 0.41 |
| 1:RA:2781:A:H5'' | 1:RA:2782:G:H5' | 2.03 | 0.41 |
| 6:RG:126:ASP:HB3 | 6:RG:128:ARG:H | 1.85 | 0.41 |
| 11:RP:96:THR:H | 11:RP:99:LEU:HD12 | 1.86 | 0.41 |
| 32:XA:620:C:C2 | 35:XD:135:LEU:HG | 2.55 | 0.41 |
| 32:XA:76:C:H42 | 32:XA:93:G:H1 | 1.67 | 0.41 |
| 32:XA:1104:G:O5' | 33:XB:111:ARG:HD2 | 2.21 | 0.41 |
| 37:XF:11:ASN:HB3 | 37:XF:14:LEU:HG | 2.03 | 0.41 |
| 38:XG:12:LEU:HD12 | 38:XG:12:LEU:H | 1.85 | 0.41 |
| 41:XJ:25:GLU:O | 41:XJ:29:ARG:HG2 | 2.20 | 0.41 |
| 44:XM:27:LYS:HA | 44:XM:27:LYS:HD3 | 1.89 | 0.41 |
| 45:YN:6:LEU:HD23 | 45:YN:23:ARG:NH2 | 2.35 | 0.41 |
| 22:Y0:68:GLU:OE1 | 22:Y0:82:ARG:NH1 | 2.53 | 0.41 |
| 23:Y1:70:VAL:O | 23:Y1:74:VAL:HG23 | 2.21 | 0.41 |
| 24:Y2:53:LEU:HD23 | 24:Y2:53:LEU:HA | 1.88 | 0.41 |
| 1:YA:1047:G:H2' | 1:YA:1110:G:H22 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:818:G:N1 | 1:YA:1188:U:OP2 | 2.33 | 0.41 |
| 1:YA:2114:A:H2' | 1:YA:2115:G:O4' | 2.21 | 0.41 |
| 1:YA:2181:G:H2' | 1:YA:2182:G:O4' | 2.20 | 0.41 |
| 1:YA:531:C:H4' | 1:YA:532:A:H5'' | 2.03 | 0.41 |
| 1:YA:721:C:H2' | 1:YA:722:A:H8 | 1.86 | 0.41 |
| 32:QA:1330:U:H2' | 32:QA:1331:G:H5' | 2.01 | 0.41 |
| 32:QA:1410:G:H2' | 32:QA:1411:C:C6 | 2.55 | 0.41 |
| 32:QA:299:G:H2' | 32:QA:300:A:C8 | 2.56 | 0.41 |
| 32:QA:302:G:O2' | 32:QA:556:C:H5'' | 2.21 | 0.41 |
| 32:QA:685:G:O2' | 32:QA:686:U:H5' | 2.19 | 0.41 |
| 32:QA:900:A:H2' | 32:QA:901:A:C8 | 2.55 | 0.41 |
| 33:QB:21:ARG:HD3 | 33:QB:21:ARG:N | 2.35 | 0.41 |
| 34:QC:82:GLU:OE1 | 34:QC:85:ARG:NH2 | 2.47 | 0.41 |
| 36:QE:69:VAL:HG21 | 36:QE:113:ALA:HB1 | 2.03 | 0.41 |
| 42:QK:84:VAL:HG21 | 42:QK:95:ILE:HD11 | 2.02 | 0.41 |
| 43:QL:83:VAL:HG13 | 43:QL:100:ILE:HG23 | 2.02 | 0.41 |
| 49:QR:42:ARG:NH2 | 49:QR:42:ARG:HA | 2.36 | 0.41 |
| 49:QR:66:LEU:O | 49:QR:70:ILE:HG13 | 2.21 | 0.41 |
| 55:QY:311:ASN:HD22 | 55:QY:314:GLN:HB2 | 1.85 | 0.41 |
| 23:R1:3:LYS:O | 23:R1:12:PRO:HD3 | 2.20 | 0.41 |
| 1:RA:1073:A:H4' | 1:RA:1074:G:OP1 | 2.21 | 0.41 |
| 1:RA:2552:2MU:H6'3 | 1:RA:2554:U:C6 | 2.56 | 0.41 |
| 4:RE:47:VAL:HG23 | 4:RE:84:PHE:O | 2.21 | 0.41 |
| 5:RF:183:VAL:O | 5:RF:187:VAL:HG23 | 2.20 | 0.41 |
| 12:RQ:30:GLY:HA2 | 12:RQ:107:ALA:HB2 | 2.03 | 0.41 |
| 32:XA:922:G:H2' | 32:XA:923:A:C8 | 2.56 | 0.41 |
| 36:XE:70:PRO:O | 36:XE:72:GLN:NE2 | 2.54 | 0.41 |
| 42:XK:84:VAL:HG11 | 42:XK:91:ARG:HH11 | 1.85 | 0.41 |
| 44:XM:80:ARG:O | 44:XM:84:ILE:HG23 | 2.20 | 0.41 |
| 50:XS:40:ILE:HB | 50:XS:67:VAL:O | 2.21 | 0.41 |
| 1:YA:1430:C:H2' | 1:YA:1431:U:C6 | 2.55 | 0.41 |
| 1:YA:1495:A:H2' | 1:YA:1496:A:C8 | 2.56 | 0.41 |
| 1:YA:2051:A:H8 | 1:YA:2051:A:OP2 | 2.03 | 0.41 |
| 1:YA:2136:C:C6 | 1:YA:2137:C:H5 | 2.38 | 0.41 |
| 1:YA:2144:U:O2' | 1:YA:2147:G:N1 | 2.49 | 0.41 |
| 1:YA:2335:A:C8 | 1:YA:2337:G:C5 | 3.08 | 0.41 |
| 1:YA:566:U:H5'' | 11:YP:29:LYS:HE3 | 2.02 | 0.41 |
| 20:YY:40:GLU:O | 20:YY:42:VAL:HG23 | 2.20 | 0.41 |
| 32:QA:1205:U:O2' | 34:QC:195:VAL:HG23 | 2.20 | 0.41 |
| 32:QA:604:G:C5 | 32:QA:635:G:C6 | 3.08 | 0.41 |
| 34:QC:59:ARG:H | 41:QJ:92:THR:CG2 | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:QE:40:ARG:NH2 | 36:QE:68:GLU:OE1 | 2.54 | 0.41 |
| 39:QH:37:ARG:HH21 | 39:QH:41:ARG:HH21 | 1.69 | 0.41 |
| 42:QK:27:ASN:OD1 | 42:QK:28:THR:N | 2.52 | 0.41 |
| 53:QV:21:A:N6 | 53:QV:46:G:H2' | 2.35 | 0.41 |
| 55:QY:247:THR:HG23 | 55:QY:254:VAL:HG12 | 2.03 | 0.41 |
| 27:R5:37:LYS:HD3 | 27:R5:37:LYS:HA | 1.90 | 0.41 |
| 1:RA:1079:C:N4 | 1:RA:1080:C:C2 | 2.82 | 0.41 |
| 1:RA:127:A:H5'' | 1:RA:128:C:O4' | 2.21 | 0.41 |
| 1:RA:1641:A:H2' | 1:RA:1642:G:O4' | 2.20 | 0.41 |
| 1:RA:2119:A:O2' | 1:RA:2120:G:H5' | 2.20 | 0.41 |
| 1:RA:2259:G:C2 | 1:RA:2282:G:N1 | 2.89 | 0.41 |
| 1:RA:361:G:O2' | 1:RA:362:U:H5' | 2.21 | 0.41 |
| 1:RA:463:G:N2 | 1:RA:466:A:OP2 | 2.43 | 0.41 |
| 1:RA:635:C:H2' | 1:RA:636:G:O4' | 2.21 | 0.41 |
| 1:RA:644:A:H4' | 1:RA:645:C:H5 | 1.84 | 0.41 |
| 1:RA:1695:G:H1' | 3:RD:8:PRO:O | 2.20 | 0.41 |
| 12:RQ:109:VAL:HG13 | 12:RQ:113:GLN:CB | 2.51 | 0.41 |
| 18:RW:37:ARG:HD3 | 18:RW:38:TYR:CE2 | 2.56 | 0.41 |
| 18:RW:65:LEU:HD23 | 18:RW:65:LEU:HA | 1.88 | 0.41 |
| 32:XA:1002:G:C4 | 32:XA:1003:G:C8 | 3.08 | 0.41 |
| 32:XA:384:G:H2' | 32:XA:385:C:C6 | 2.55 | 0.41 |
| 34:XC:12:LEU:O | 45:XN:57:ARG:NH2 | 2.41 | 0.41 |
| 48:XQ:19:VAL:HG23 | 48:XQ:44:ALA:HB3 | 2.02 | 0.41 |
| 53:XV:4:G:O2' | 53:XV:5:G:H8 | 2.02 | 0.41 |
| 1:YA:1059:G:N2 | 1:YA:1079:C:N3 | 2.69 | 0.41 |
| 1:YA:2122:U:H2' | 1:YA:2123:G:C8 | 2.56 | 0.41 |
| 1:YA:2869:G:H2' | 1:YA:2870:C:O4' | 2.21 | 0.41 |
| 1:YA:7:G:H2' | 1:YA:8:A:H8 | 1.84 | 0.41 |
| 5:YF:33:LEU:HB3 | 11:YP:6:LEU:HD21 | 2.02 | 0.41 |
| 8:YI:62:LYS:HG2 | 8:YI:133:HIS:CD2 | 2.56 | 0.41 |
| 17:YV:40:LEU:HB2 | 17:YV:46:VAL:HG12 | 2.01 | 0.41 |
| 21:YZ:126:VAL:CG1 | 21:YZ:161:VAL:HG13 | 2.50 | 0.41 |
| 32:QA:1225:A:H2' | 32:QA:1226:C:C5 | 2.56 | 0.41 |
| 32:QA:519:C:OP2 | 43:QL:50:SER:OG | 2.23 | 0.41 |
| 32:QA:1148:U:O4' | 40:QI:16:ARG:HD2 | 2.20 | 0.41 |
| 1:RA:1045:A:H8 | 1:RA:1047:G:N3 | 2.18 | 0.41 |
| 1:RA:2136:C:C6 | 1:RA:2137:C:H5 | 2.39 | 0.41 |
| 1:RA:2734:A:H2' | 1:RA:2735:G:O4' | 2.21 | 0.41 |
| 1:RA:2752:C:H2' | 1:RA:2753:A:O4' | 2.21 | 0.41 |
| 1:RA:2852:G:H2' | 1:RA:2853:C:O4' | 2.20 | 0.41 |
| 1:RA:588:U:H1' | 5:RF:90:PHE:CG | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:RG:133:LEU:HD11 | 6:RG:157:ILE:HD12 | 2.03 | 0.41 |
| 6:RG:79:ASN:OD1 | 6:RG:79:ASN:N | 2.53 | 0.41 |
| 9:RN:14:VAL:HG11 | 9:RN:138:LEU:HD12 | 2.01 | 0.41 |
| 17:RV:76:LYS:HB2 | 17:RV:81:TYR:HB3 | 2.03 | 0.41 |
| 32:XA:1084:G:H5' | 32:XA:1102:A:OP2 | 2.21 | 0.41 |
| 32:XA:1216:G:H5'' | 45:YN:5:ALA:HB2 | 2.03 | 0.41 |
| 32:XA:155:C:H2' | 32:XA:156:G:O4' | 2.21 | 0.41 |
| 32:XA:691:G:H1' | 32:XA:696:A:N6 | 2.35 | 0.41 |
| 23:Y1:51:VAL:HG11 | 23:Y1:74:VAL:CG2 | 2.51 | 0.41 |
| 1:YA:1083:U:H5'' | 1:YA:1084:A:OP1 | 2.21 | 0.41 |
| 1:YA:1301:A:C8 | 1:YA:1303:G:C8 | 3.09 | 0.41 |
| 1:YA:2330:G:H2' | 1:YA:2331:G:O4' | 2.21 | 0.41 |
| 1:YA:36:G:O2' | 1:YA:450:G:H2' | 2.21 | 0.41 |
| 2:YB:43:C:H5'' | 26:Y4:1:MET:HG2 | 2.02 | 0.41 |
| 4:YE:47:VAL:O | 4:YE:80:GLU:HA | 2.21 | 0.41 |
| 1:YA:2786:U:O2 | 4:YE:62:PRO:HB3 | 2.20 | 0.41 |
| 6:YG:43:LEU:HB3 | 6:YG:44:GLY:H | 1.68 | 0.41 |
| 9:YN:99:LEU:HD23 | 9:YN:99:LEU:HA | 1.85 | 0.41 |
| 21:YZ:14:LYS:HB3 | 21:YZ:14:LYS:HE2 | 1.79 | 0.41 |
| 32:QA:1277:C:HO2' | 32:QA:1279:A:H8 | 1.64 | 0.41 |
| 32:QA:160:A:H2' | 32:QA:161:A:O4' | 2.20 | 0.41 |
| 32:QA:486:U:H2' | 32:QA:487:A:C8 | 2.56 | 0.41 |
| 34:QC:181:ASN:HB3 | 34:QC:205:GLY:O | 2.21 | 0.41 |
| 36:QE:116:THR:HG23 | 36:QE:117:ASP:OD2 | 2.21 | 0.41 |
| 1:RA:725:G:C6 | 1:RA:726:G:N1 | 2.89 | 0.41 |
| 1:RA:746:A:H2' | 1:RA:2612:C:H5'' | 2.03 | 0.41 |
| 2:RB:24:G:N7 | 2:RB:56:G:H2' | 2.36 | 0.41 |
| 2:RB:95:C:H2' | 2:RB:96:U:C6 | 2.56 | 0.41 |
| 3:RD:132:PRO:HD3 | 3:RD:190:TYR:CZ | 2.56 | 0.41 |
| 4:RE:28:ALA:HB3 | 4:RE:93:VAL:HG12 | 2.03 | 0.41 |
| 10:RO:8:LEU:HD13 | 10:RO:82:ASN:HB3 | 2.03 | 0.41 |
| 12:RQ:32:TYR:OH | 12:RQ:111:GLU:OE1 | 2.22 | 0.41 |
| 15:YT:41:ARG:NH2 | 32:XA:346:G:OP1 | 2.38 | 0.41 |
| 32:XA:540:G:C6 | 32:XA:541:G:C5 | 3.09 | 0.41 |
| 32:XA:730:G:C5 | 32:XA:731:G:H1' | 2.56 | 0.41 |
| 36:XE:110:LEU:HD13 | 36:XE:118:ILE:HG21 | 2.03 | 0.41 |
| 39:XH:14:ARG:O | 39:XH:18:ARG:HD3 | 2.21 | 0.41 |
| 42:XK:82:VAL:HB | 42:XK:108:ILE:HG12 | 2.03 | 0.41 |
| 26:Y4:61:ARG:HG2 | 50:XS:42:PRO:CG | 2.51 | 0.41 |
| 1:YA:1268:A:H2' | 1:YA:1269:A:O4' | 2.21 | 0.41 |
| 1:YA:207:A:H2' | 1:YA:208:C:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:YA:954:G:O2' | 1:YA:2274:A:N1 | 2.44 | 0.41 |
| 1:YA:24:G:H2' | 1:YA:25:U:O4' | 2.21 | 0.41 |
| 1:YA:972:G:C6 | 1:YA:973:A:C6 | 3.09 | 0.41 |
| 6:YG:114:ILE:HA | 6:YG:136:ARG:HH22 | 1.86 | 0.41 |
| 32:QA:434:U:H2' | 32:QA:435:C:C6 | 2.56 | 0.41 |
| 48:QQ:86:GLU:O | 48:QQ:90:ILE:HG12 | 2.21 | 0.41 |
| 55:QY:233:GLY:HA3 | 55:QY:237:VAL:CG2 | 2.50 | 0.41 |
| 55:QY:341:ILE:O | 55:QY:345:ILE:HG13 | 2.21 | 0.41 |
| 28:R6:8:LYS:HD3 | 30:R8:34:TRP:HB3 | 2.03 | 0.41 |
| 1:RA:1274:A:N3 | 1:RA:1297:C:H1' | 2.36 | 0.41 |
| 1:RA:2112:G:H2' | 1:RA:2113:U:C6 | 2.56 | 0.41 |
| 1:RA:2745:C:H2' | 1:RA:2746:U:O4' | 2.21 | 0.41 |
| 1:RA:286:C:H2' | 1:RA:287:C:C6 | 2.56 | 0.41 |
| 8:RI:92:VAL:CG1 | 8:RI:120:ILE:HB | 2.51 | 0.41 |
| 12:RQ:137:TYR:O | 12:RQ:141:GLN:HG2 | 2.21 | 0.41 |
| 32:XA:1144:G:C6 | 32:XA:1145:C:C4 | 3.09 | 0.41 |
| 32:XA:1502:A:C8 | 32:XA:1505:G:N2 | 2.89 | 0.41 |
| 32:XA:411:A:O2' | 32:XA:413:G:H5' | 2.20 | 0.41 |
| 55:XY:183:ARG:HA | 55:XY:200:ALA:HB2 | 2.02 | 0.41 |
| 55:XY:187:VAL:HG13 | 55:XY:196:ILE:HD13 | 2.03 | 0.41 |
| 26:Y4:8:LYS:HE2 | 26:Y4:8:LYS:HB3 | 1.85 | 0.41 |
| 1:YA:1073:A:H4' | 1:YA:1074:G:OP1 | 2.22 | 0.41 |
| 1:YA:2328:A:H2' | 1:YA:2329:G:C8 | 2.56 | 0.41 |
| 1:YA:2747:G:OP1 | 7:YH:138:LYS:NZ | 2.51 | 0.41 |
| 1:YA:969:U:H2' | 1:YA:970:C:C6 | 2.56 | 0.41 |
| 2:YB:73:A:C4 | 2:YB:105:A:C2 | 3.09 | 0.41 |
| 13:YR:87:TYR:OH | 13:YR:117:VAL:O | 2.26 | 0.41 |
| 18:YW:9:TYR:HA | 18:YW:100:THR:HG23 | 2.01 | 0.41 |
| 32:QA:1081:G:H8 | 32:QA:1081:G:O5' | 2.04 | 0.40 |
| 32:QA:102:G:O2' | 32:QA:151:A:N3 | 2.43 | 0.40 |
| 32:QA:743:U:H2' | 32:QA:744:C:C6 | 2.56 | 0.40 |
| 33:QB:19:HIS:HE1 | 33:QB:206:ASP:OD2 | 2.04 | 0.40 |
| 32:QA:4:U:C4 | 39:QH:105:ARG:HD3 | 2.56 | 0.40 |
| 41:QJ:4:ILE:N | 41:QJ:100:THR:HG22 | 2.36 | 0.40 |
| 47:QP:5:ARG:HH21 | 47:QP:24:ALA:HA | 1.85 | 0.40 |
| 24:R2:53:LEU:HD23 | 24:R2:53:LEU:HA | 1.89 | 0.40 |
| 19:RX:60:ARG:NH1 | 29:R7:47:ARG:HH22 | 2.19 | 0.40 |
| 1:RA:1469:A:H2' | 1:RA:1470:G:O4' | 2.22 | 0.40 |
| 1:RA:2134:A:C5 | 1:RA:2157:G:H5' | 2.56 | 0.40 |
| 1:RA:2647:U:H2' | 1:RA:2648:C:C6 | 2.56 | 0.40 |
| 1:RA:2749:A:C6 | 1:RA:2750:A:C6 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:RA:27:G:O2' | 1:RA:28:A:OP2 | 2.36 | 0.40 |
| 1:RA:443:A:H1' | 1:RA:1201:C:O4' | 2.21 | 0.40 |
| 7:RH:20:ALA:HB1 | 7:RH:21:PRO:HD2 | 2.01 | 0.40 |
| 9:RN:42:TRP:CH2 | 9:RN:44:PRO:HB3 | 2.56 | 0.40 |
| 12:RQ:111:GLU:O | 12:RQ:115:MET:HG2 | 2.21 | 0.40 |
| 13:RR:54:LEU:HD12 | 13:RR:54:LEU:HA | 1.98 | 0.40 |
| 21:RZ:125:LEU:HG | 21:RZ:164:ALA:HB3 | 2.02 | 0.40 |
| 32:XA:337:C:H2' | 32:XA:338:A:C8 | 2.56 | 0.40 |
| 32:XA:411:A:OP1 | 35:XD:30:LYS:NZ | 2.45 | 0.40 |
| 32:XA:501:C:H1' | 32:XA:549:C:H1' | 2.03 | 0.40 |
| 38:XG:108:ALA:O | 38:XG:119:ARG:HD2 | 2.21 | 0.40 |
| 32:XA:663:A:H5" | 49:XR:61:LYS:NZ | 2.36 | 0.40 |
| 1:YA:1291:C:H2' | 1:YA:1292:U:C6 | 2.56 | 0.40 |
| 1:YA:2505:G:O6 | 1:YA:2576:G:H2' | 2.20 | 0.40 |
| 1:YA:656:G:H2' | 1:YA:657:U:O4' | 2.22 | 0.40 |
| 2:YB:13:A:O2' | 2:YB:14:U:H3' | 2.21 | 0.40 |
| 3:YD:232:PRO:HB3 | 3:YD:244:ARG:CZ | 2.51 | 0.40 |
| 7:YH:13:LYS:HA | 7:YH:14:GLY:HA2 | 1.79 | 0.40 |
| 14:YS:49:VAL:HG21 | 14:YS:77:ALA:HA | 2.03 | 0.40 |
| 2:YB:77:U:OP1 | 21:YZ:19:ARG:NH2 | 2.54 | 0.40 |
| 32:QA:1353:G:C2 | 32:QA:1370:G:C2 | 3.09 | 0.40 |
| 32:QA:1417:G:O2' | 32:QA:1483:A:N6 | 2.51 | 0.40 |
| 35:QD:31:CYS:O | 35:QD:35:ARG:HG3 | 2.22 | 0.40 |
| 38:QG:102:ARG:O | 38:QG:106:GLN:HG3 | 2.22 | 0.40 |
| 43:QL:124:LYS:HA | 43:QL:125:PRO:HD3 | 1.94 | 0.40 |
| 32:QA:127:G:O2' | 48:QQ:2:PRO:O | 2.37 | 0.40 |
| 55:QY:143:ARG:NE | 55:QY:143:ARG:HA | 2.36 | 0.40 |
| 28:R6:8:LYS:HG2 | 30:R8:34:TRP:CD1 | 2.56 | 0.40 |
| 1:RA:1431:U:H2' | 1:RA:1432:C:C6 | 2.56 | 0.40 |
| 1:RA:1689:A:H4' | 32:QA:1475:G:H4' | 2.03 | 0.40 |
| 1:RA:1790:C:H2' | 1:RA:1791:A:C5 | 2.56 | 0.40 |
| 1:RA:2114:A:H2' | 1:RA:2115:G:O4' | 2.21 | 0.40 |
| 1:RA:2359:C:H2' | 1:RA:2360:A:O4' | 2.20 | 0.40 |
| 1:RA:2552:2MU:H6 | 1:RA:2552:2MU:O5' | 2.21 | 0.40 |
| 1:RA:662:G:H5' | 11:RP:14:LYS:O | 2.22 | 0.40 |
| 32:XA:149:A:H2' | 32:XA:150:C:C6 | 2.56 | 0.40 |
| 32:XA:1516:G:H2' | 32:XA:1518:MA6:OP2 | 2.22 | 0.40 |
| 32:XA:561:U:HO2' | 32:XA:562:C:P | 2.44 | 0.40 |
| 32:XA:598:U:H4' | 39:XH:94:TYR:CD2 | 2.57 | 0.40 |
| 32:XA:778:G:H2' | 32:XA:779:C:O4' | 2.21 | 0.40 |
| 33:XB:20:GLU:HB3 | 33:XB:21:ARG:H | 1.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:XC:125:GLU:OE1 | 34:XC:190:ARG:HD3 | 2.20 | 0.40 |
| 55:XY:274:LEU:HA | 55:XY:274:LEU:HD23 | 1.94 | 0.40 |
| 23:Y1:54:ALA:HB1 | 23:Y1:83:GLU:HG3 | 2.02 | 0.40 |
| 1:YA:2526:G:O2' | 31:Y9:1:MET:HB2 | 2.21 | 0.40 |
| 1:YA:2370:G:C6 | 1:YA:2371:G:C6 | 3.09 | 0.40 |
| 1:YA:2522:U:O2' | 1:YA:2647:U:OP1 | 2.30 | 0.40 |
| 1:YA:2660:A:H2' | 1:YA:2661:G:O4' | 2.22 | 0.40 |
| 1:YA:644:A:H4' | 1:YA:645:C:H5 | 1.86 | 0.40 |
| 1:YA:674:G:O2' | 5:YF:74:ARG:HD3 | 2.21 | 0.40 |
| 1:YA:686:G:N2 | 1:YA:788:A:H61 | 2.20 | 0.40 |
| 2:YB:75:G:N3 | 21:YZ:85:HIS:CE1 | 2.90 | 0.40 |
| 5:YF:110:LEU:HD13 | 5:YF:202:PHE:HE1 | 1.87 | 0.40 |
| 14:YS:23:ARG:NH1 | 14:YS:85:VAL:O | 2.54 | 0.40 |
| 21:YZ:108:PRO:HA | 21:YZ:142:SER:HA | 2.03 | 0.40 |
| 32:QA:1035:A:H8 | 32:QA:1035:A:O5' | 2.04 | 0.40 |
| 32:QA:1312:G:N7 | 50:QS:2:PRO:HD2 | 2.37 | 0.40 |
| 32:QA:195:A:C6 | 32:QA:196:A:N1 | 2.90 | 0.40 |
| 32:QA:429:U:H3' | 35:QD:9:CYS:SG | 2.61 | 0.40 |
| 48:QQ:22:LEU:HD13 | 48:QQ:41:LYS:HG3 | 2.03 | 0.40 |
| 53:QV:16:C:O2' | 53:QV:61:C:OP1 | 2.36 | 0.40 |
| 1:RA:1614:A:P | 1:RA:1614:A:H8 | 2.45 | 0.40 |
| 1:RA:1913:A:N7 | 32:QA:1493:A:O2' | 2.43 | 0.40 |
| 1:RA:2144:U:H1' | 1:RA:2147:G:O6 | 2.21 | 0.40 |
| 1:RA:2163:C:H5'' | 1:RA:2164:C:OP2 | 2.22 | 0.40 |
| 1:RA:2643:G:H2' | 1:RA:2644:G:O4' | 2.21 | 0.40 |
| 1:RA:900:A:H2' | 1:RA:901:A:O4' | 2.21 | 0.40 |
| 3:RD:72:LYS:HG3 | 3:RD:103:ARG:HH22 | 1.86 | 0.40 |
| 5:RF:150:GLY:HA2 | 5:RF:172:TRP:CD2 | 2.56 | 0.40 |
| 5:RF:20:LEU:HD13 | 5:RF:21:ALA:N | 2.37 | 0.40 |
| 10:RO:64:ARG:NH2 | 10:RO:99:PHE:O | 2.55 | 0.40 |
| 11:RP:83:VAL:HG12 | 11:RP:112:LEU:HD21 | 2.02 | 0.40 |
| 21:RZ:28:MET:HA | 21:RZ:88:PHE:O | 2.21 | 0.40 |
| 33:XB:92:TYR:CE1 | 33:XB:94:ASN:HB2 | 2.57 | 0.40 |
| 35:XD:111:ALA:HB2 | 35:XD:120:LEU:HD12 | 2.03 | 0.40 |
| 41:XJ:32:ALA:HB1 | 41:XJ:33:GLN:CD | 2.42 | 0.40 |
| 55:XY:223:ARG:NH1 | 55:XY:225:ASP:OD2 | 2.54 | 0.40 |
| 1:YA:1075:C:N4 | 1:YA:1077:A:C5 | 2.89 | 0.40 |
| 1:YA:55:G:O2' | 1:YA:127:A:N1 | 2.38 | 0.40 |
| 1:YA:2319:G:H1 | 14:YS:3:ARG:NH2 | 2.19 | 0.40 |
| 1:YA:2364:C:H2' | 1:YA:2365:G:O4' | 2.21 | 0.40 |
| 1:YA:2345:G:N3 | 1:YA:2381:C:H2' | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:YA:322:A:OP1 | 5:YF:168:ARG:HD2 | 2.21 | 0.40 |
| 1:YA:639:U:H2' | 1:YA:640:C:C6 | 2.56 | 0.40 |
| 1:YA:64:A:O3' | 19:YX:71:GLY:HA3 | 2.22 | 0.40 |
| 2:YB:22:U:H2' | 2:YB:23:G:C8 | 2.56 | 0.40 |
| 1:YA:784:A:N6 | 3:YD:229:VAL:HG11 | 2.36 | 0.40 |
| 32:QA:1020:U:H2' | 32:QA:1021:G:H8 | 1.84 | 0.40 |
| 32:QA:1030(D):G:H2' | 32:QA:1030(E):A:H8 | 1.86 | 0.40 |
| 32:QA:1030(D):G:C8 | 32:QA:1031:G:N2 | 2.89 | 0.40 |
| 32:QA:1183:A:H3' | 32:QA:1184:G:H5'' | 2.02 | 0.40 |
| 32:QA:1263:C:H2' | 32:QA:1264:C:C6 | 2.55 | 0.40 |
| 37:QF:45:LEU:HD12 | 37:QF:59:TYR:CD2 | 2.56 | 0.40 |
| 44:QM:88:ARG:HG3 | 44:QM:98:VAL:HG11 | 2.03 | 0.40 |
| 47:QP:57:ARG:NH2 | 47:QP:78:GLY:O | 2.54 | 0.40 |
| 48:QQ:6:LEU:O | 48:QQ:58:GLU:HA | 2.22 | 0.40 |
| 23:R1:67:ILE:N | 23:R1:68:PRO:HD2 | 2.37 | 0.40 |
| 1:RA:2181:G:H2' | 1:RA:2182:G:O4' | 2.22 | 0.40 |
| 1:RA:1637:A:H4' | 1:RA:2711:A:O2' | 2.21 | 0.40 |
| 1:RA:489:G:N7 | 18:RW:49:LYS:NZ | 2.69 | 0.40 |
| 1:RA:1569:A:H5' | 3:RD:61:LEU:HD11 | 2.02 | 0.40 |
| 11:RP:138:LEU:HD23 | 11:RP:145:PRO:HB3 | 2.03 | 0.40 |
| 1:RA:1653:G:C6 | 13:RR:9:LYS:HB2 | 2.56 | 0.40 |
| 21:RZ:24:LEU:HD21 | 21:RZ:86:VAL:HG13 | 2.03 | 0.40 |
| 32:XA:1014:A:C2 | 32:XA:1219:U:H1' | 2.56 | 0.40 |
| 32:XA:1410:G:H2' | 32:XA:1411:C:C6 | 2.56 | 0.40 |
| 32:XA:186:C:H5' | 51:XT:78:ALA:HB1 | 2.03 | 0.40 |
| 33:XB:55:PHE:HD1 | 33:XB:55:PHE:HA | 1.76 | 0.40 |
| 40:XI:7:THR:O | 40:XI:83:ARG:HD2 | 2.22 | 0.40 |
| 32:XA:449:C:O2 | 47:XP:42:ARG:HD2 | 2.21 | 0.40 |
| 23:Y1:53:VAL:HG22 | 23:Y1:74:VAL:HG13 | 2.02 | 0.40 |
| 1:YA:1180:C:H2' | 1:YA:1181:C:C6 | 2.57 | 0.40 |
| 1:YA:1638:C:H2' | 1:YA:1639:U:O4' | 2.22 | 0.40 |
| 1:YA:1847:A:H3' | 1:YA:1848:A:H5' | 2.02 | 0.40 |
| 1:YA:2114:A:H3' | 1:YA:2115:G:H8 | 1.85 | 0.40 |
| 1:YA:2752:C:H2' | 1:YA:2753:A:O4' | 2.21 | 0.40 |
| 1:YA:372:G:H8 | 23:Y1:65:SER:O | 2.04 | 0.40 |
| 4:YE:144:ARG:HB3 | 4:YE:145:LYS:H | 1.53 | 0.40 |
| 5:YF:40:GLN:NE2 | 5:YF:182:ASN:HB2 | 2.36 | 0.40 |
| 1:YA:588:U:H1' | 5:YF:90:PHE:CG | 2.56 | 0.40 |
| 13:YR:13:HIS:CE1 | 13:YR:16:HIS:HB2 | 2.56 | 0.40 |
| 16:YU:104:GLN:CD | 16:YU:104:GLN:H | 2.25 | 0.40 |
| 20:YY:56:PRO:O | 20:YY:57:GLN:HB2 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:QA:1499:A:H1' | 32:QA:1520:G:H5' | 2.02 | 0.40 |
| 32:QA:126:G:O2' | 32:QA:635:G:O4' | 2.35 | 0.40 |
| 46:QO:21:ASP:OD1 | 46:QO:24:SER:HB3 | 2.22 | 0.40 |
| 1:RA:2344:U:OP2 | 28:R6:37:ARG:HB2 | 2.21 | 0.40 |
| 1:RA:1043:C:HO2' | 1:RA:1048:A:HO2' | 1.67 | 0.40 |
| 1:RA:1050:A:C2 | 1:RA:1051:G:C5 | 3.09 | 0.40 |
| 1:RA:1083:U:H5'' | 1:RA:1084:A:OP1 | 2.22 | 0.40 |
| 1:RA:115:C:HO2' | 1:RA:127:A:HO2' | 1.70 | 0.40 |
| 1:RA:1392:A:C6 | 1:RA:1393:A:C6 | 3.09 | 0.40 |
| 1:RA:1410:G:H2' | 1:RA:1411:C:H6 | 1.85 | 0.40 |
| 1:RA:1495:A:H2' | 1:RA:1496:A:C8 | 2.56 | 0.40 |
| 1:RA:1510:G:H2' | 1:RA:1511:C:C6 | 2.57 | 0.40 |
| 1:RA:2311:A:H3' | 1:RA:2312:U:C6 | 2.56 | 0.40 |
| 1:RA:2802:G:H2' | 1:RA:2803:C:O4' | 2.22 | 0.40 |
| 1:RA:350:U:H2' | 1:RA:351:G:O4' | 2.21 | 0.40 |
| 1:RA:752:A:H3' | 29:R7:1:MET:CE | 2.52 | 0.40 |
| 1:RA:783:A:O2' | 1:RA:785:G:OP1 | 2.31 | 0.40 |
| 3:RD:70:TRP:HB3 | 3:RD:190:TYR:CE1 | 2.56 | 0.40 |
| 4:RE:119:ARG:HG2 | 4:RE:120:TRP:CE2 | 2.57 | 0.40 |
| 19:RX:12:VAL:HG22 | 19:RX:29:TRP:CE2 | 2.56 | 0.40 |
| 32:XA:1070:U:H2' | 32:XA:1071:C:C6 | 2.57 | 0.40 |
| 32:XA:1143:G:H2' | 32:XA:1144:G:H8 | 1.86 | 0.40 |
| 32:XA:719:C:H3' | 32:XA:720:C:C6 | 2.56 | 0.40 |
| 32:XA:857:C:H2' | 32:XA:858:G:O4' | 2.20 | 0.40 |
| 35:XD:10:ARG:HB2 | 35:XD:40:PRO:HG3 | 2.04 | 0.40 |
| 32:XA:404:U:H5' | 35:XD:122:ARG:HD3 | 2.03 | 0.40 |
| 37:XF:61:LEU:HD23 | 37:XF:63:TYR:OH | 2.21 | 0.40 |
| 40:XI:6:GLY:HA3 | 40:XI:83:ARG:HB2 | 2.03 | 0.40 |
| 44:XM:89:GLY:O | 44:XM:93:ARG:HG3 | 2.22 | 0.40 |
| 47:XP:3:LYS:O | 47:XP:21:VAL:HA | 2.22 | 0.40 |
| 32:XA:1236:A:OP2 | 52:XU:3:LYS:HD3 | 2.22 | 0.40 |
| 1:YA:1359:A:N1 | 1:YA:1372:U:O4 | 2.54 | 0.40 |
| 1:YA:1479:G:H5'' | 1:YA:1560:G:H4' | 2.02 | 0.40 |
| 1:YA:2118:U:H5 | 1:YA:2148:G:H1' | 1.86 | 0.40 |
| 1:YA:2144:U:O3' | 1:YA:2145:C:H2' | 2.22 | 0.40 |
| 1:YA:2282:G:OP1 | 1:YA:2283:C:H1' | 2.21 | 0.40 |
| 2:YB:28:C:H2' | 2:YB:29:A:O4' | 2.21 | 0.40 |
| 11:YP:6:LEU:HA | 11:YP:6:LEU:HD23 | 1.79 | 0.40 |
| 5:YF:34:TRP:CZ3 | 11:YP:8:PRO:HB3 | 2.57 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------------|--------------------------|-------------------|
| 24:R2:46:GLN:OE1 | 1:YA:277:C:O2'[3_555] | 2.14 | 0.06 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3 | RD | 273/276 (99%) | 261 (96%) | 12 (4%) | 0 | 100 | 100 |
| 3 | YD | 273/276 (99%) | 262 (96%) | 11 (4%) | 0 | 100 | 100 |
| 4 | RE | 202/206 (98%) | 195 (96%) | 6 (3%) | 1 (0%) | 34 | 78 |
| 4 | YE | 202/206 (98%) | 195 (96%) | 7 (4%) | 0 | 100 | 100 |
| 5 | RF | 201/210 (96%) | 197 (98%) | 4 (2%) | 0 | 100 | 100 |
| 5 | YF | 201/210 (96%) | 196 (98%) | 3 (2%) | 2 (1%) | 19 | 65 |
| 6 | RG | 179/182 (98%) | 166 (93%) | 12 (7%) | 1 (1%) | 30 | 75 |
| 6 | YG | 179/182 (98%) | 170 (95%) | 8 (4%) | 1 (1%) | 30 | 75 |
| 7 | RH | 172/180 (96%) | 167 (97%) | 5 (3%) | 0 | 100 | 100 |
| 7 | YH | 171/180 (95%) | 164 (96%) | 7 (4%) | 0 | 100 | 100 |
| 8 | RI | 145/148 (98%) | 135 (93%) | 10 (7%) | 0 | 100 | 100 |
| 8 | YI | 144/148 (97%) | 137 (95%) | 7 (5%) | 0 | 100 | 100 |
| 9 | RN | 138/140 (99%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 9 | YN | 138/140 (99%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 10 | RO | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 10 | YO | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 11 | RP | 147/150 (98%) | 142 (97%) | 4 (3%) | 1 (1%) | 26 | 72 |
| 11 | YP | 147/150 (98%) | 142 (97%) | 4 (3%) | 1 (1%) | 26 | 72 |
| 12 | RQ | 139/141 (99%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 12 | YQ | 139/141 (99%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 13 | RR | 116/118 (98%) | 114 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 13 | YR | 116/118 (98%) | 114 (98%) | 2 (2%) | 0 | 100 | 100 |
| 14 | RS | 108/112 (96%) | 104 (96%) | 3 (3%) | 1 (1%) | 21 | 67 |
| 14 | YS | 108/112 (96%) | 105 (97%) | 3 (3%) | 0 | 100 | 100 |
| 15 | RT | 129/146 (88%) | 124 (96%) | 5 (4%) | 0 | 100 | 100 |
| 15 | YT | 129/146 (88%) | 125 (97%) | 4 (3%) | 0 | 100 | 100 |
| 16 | RU | 114/118 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | YU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 17 | RV | 99/101 (98%) | 96 (97%) | 2 (2%) | 1 (1%) | 19 | 65 |
| 17 | YV | 99/101 (98%) | 96 (97%) | 2 (2%) | 1 (1%) | 19 | 65 |
| 18 | RW | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 18 | YW | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | RX | 93/96 (97%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | YX | 93/96 (97%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 20 | RY | 105/110 (96%) | 99 (94%) | 6 (6%) | 0 | 100 | 100 |
| 20 | YY | 105/110 (96%) | 102 (97%) | 3 (3%) | 0 | 100 | 100 |
| 21 | RZ | 187/206 (91%) | 182 (97%) | 5 (3%) | 0 | 100 | 100 |
| 21 | YZ | 187/206 (91%) | 181 (97%) | 6 (3%) | 0 | 100 | 100 |
| 22 | R0 | 75/85 (88%) | 73 (97%) | 2 (3%) | 0 | 100 | 100 |
| 22 | Y0 | 75/85 (88%) | 73 (97%) | 2 (3%) | 0 | 100 | 100 |
| 23 | R1 | 95/98 (97%) | 94 (99%) | 0 | 1 (1%) | 17 | 62 |
| 23 | Y1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 17 | 62 |
| 24 | R2 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 24 | Y2 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | R3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 25 | Y3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 26 | R4 | 67/71 (94%) | 56 (84%) | 7 (10%) | 4 (6%) | 2 | 16 |
| 26 | Y4 | 67/71 (94%) | 55 (82%) | 9 (13%) | 3 (4%) | 3 | 24 |
| 27 | R5 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 27 | Y5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 28 | R6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 28 | Y6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29 | R7 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 29 | Y7 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 30 | R8 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 30 | Y8 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 31 | R9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 31 | Y9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 33 | QB | 229/256 (90%) | 201 (88%) | 24 (10%) | 4 (2%) | 11 | 52 |
| 33 | XB | 229/256 (90%) | 205 (90%) | 19 (8%) | 5 (2%) | 8 | 45 |
| 34 | QC | 204/239 (85%) | 190 (93%) | 14 (7%) | 0 | 100 | 100 |
| 34 | XC | 204/239 (85%) | 189 (93%) | 15 (7%) | 0 | 100 | 100 |
| 35 | QD | 206/209 (99%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 35 | XD | 206/209 (99%) | 199 (97%) | 7 (3%) | 0 | 100 | 100 |
| 36 | QE | 146/162 (90%) | 144 (99%) | 2 (1%) | 0 | 100 | 100 |
| 36 | XE | 146/162 (90%) | 144 (99%) | 2 (1%) | 0 | 100 | 100 |
| 37 | QF | 98/101 (97%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 37 | XF | 98/101 (97%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 38 | QG | 153/156 (98%) | 151 (99%) | 2 (1%) | 0 | 100 | 100 |
| 38 | XG | 153/156 (98%) | 149 (97%) | 3 (2%) | 1 (1%) | 26 | 72 |
| 39 | QH | 135/138 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 39 | XH | 135/138 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 40 | QI | 125/128 (98%) | 116 (93%) | 9 (7%) | 0 | 100 | 100 |
| 40 | XI | 124/128 (97%) | 113 (91%) | 9 (7%) | 2 (2%) | 12 | 54 |
| 41 | QJ | 95/105 (90%) | 83 (87%) | 8 (8%) | 4 (4%) | 3 | 26 |
| 41 | XJ | 94/105 (90%) | 84 (89%) | 8 (8%) | 2 (2%) | 9 | 46 |
| 42 | QK | 112/129 (87%) | 105 (94%) | 6 (5%) | 1 (1%) | 21 | 67 |
| 42 | XK | 112/129 (87%) | 106 (95%) | 6 (5%) | 0 | 100 | 100 |
| 43 | QL | 119/132 (90%) | 117 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | XL | 119/132 (90%) | 116 (98%) | 3 (2%) | 0 | 100 | 100 |
| 44 | QM | 114/126 (90%) | 105 (92%) | 7 (6%) | 2 (2%) | 11 | 51 |
| 44 | XM | 112/126 (89%) | 105 (94%) | 6 (5%) | 1 (1%) | 21 | 67 |
| 45 | QN | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 45 | XN | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 46 | QO | 86/89 (97%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |
| 46 | XO | 86/89 (97%) | 82 (95%) | 4 (5%) | 0 | 100 | 100 |
| 47 | QP | 80/88 (91%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 47 | XP | 80/88 (91%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 48 | QQ | 97/105 (92%) | 94 (97%) | 2 (2%) | 1 (1%) | 19 | 65 |
| 48 | XQ | 97/105 (92%) | 95 (98%) | 2 (2%) | 0 | 100 | 100 |
| 49 | QR | 66/88 (75%) | 66 (100%) | 0 | 0 | 100 | 100 |
| 49 | XR | 66/88 (75%) | 65 (98%) | 1 (2%) | 0 | 100 | 100 |
| 50 | QS | 81/93 (87%) | 78 (96%) | 2 (2%) | 1 (1%) | 16 | 60 |
| 50 | XS | 81/93 (87%) | 77 (95%) | 4 (5%) | 0 | 100 | 100 |
| 51 | QT | 94/106 (89%) | 88 (94%) | 5 (5%) | 1 (1%) | 17 | 62 |
| 51 | XT | 96/106 (91%) | 89 (93%) | 5 (5%) | 2 (2%) | 9 | 46 |
| 52 | QU | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 52 | XU | 21/27 (78%) | 18 (86%) | 2 (10%) | 1 (5%) | 3 | 22 |
| 55 | QY | 255/360 (71%) | 224 (88%) | 17 (7%) | 14 (6%) | 2 | 18 |
| 55 | XY | 256/360 (71%) | 222 (87%) | 25 (10%) | 9 (4%) | 4 | 31 |
| All | All | 11925/12848 (93%) | 11396 (96%) | 459 (4%) | 70 (1%) | 30 | 75 |

All (70) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | R4 | 49 | PHE |
| 33 | QB | 16 | HIS |
| 33 | QB | 22 | LYS |
| 51 | QT | 95 | ALA |
| 55 | QY | 215 | PRO |
| 55 | QY | 217 | ILE |
| 55 | QY | 241 | ASP |
| 55 | QY | 306 | ARG |
| 55 | QY | 322 | ILE |
| 23 | Y1 | 3 | LYS |
| 33 | XB | 17 | PHE |
| 33 | XB | 20 | GLU |
| 33 | XB | 124 | SER |
| 40 | XI | 44 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | XI | 54 | ASP |
| 55 | XY | 105 | PRO |
| 6 | RG | 51 | ARG |
| 14 | RS | 60 | GLY |
| 26 | R4 | 45 | GLY |
| 26 | R4 | 47 | GLN |
| 26 | R4 | 55 | ARG |
| 41 | QJ | 31 | GLY |
| 41 | QJ | 78 | ASN |
| 55 | QY | 105 | PRO |
| 55 | QY | 121 | GLY |
| 55 | QY | 220 | ALA |
| 55 | QY | 299 | GLY |
| 5 | YF | 21 | ALA |
| 6 | YG | 81 | LYS |
| 26 | Y4 | 60 | GLN |
| 33 | XB | 10 | LEU |
| 44 | XM | 67 | GLU |
| 51 | XT | 95 | ALA |
| 55 | XY | 322 | ILE |
| 33 | QB | 17 | PHE |
| 41 | QJ | 79 | ARG |
| 33 | XB | 125 | PRO |
| 41 | XJ | 78 | ASN |
| 41 | XJ | 79 | ARG |
| 55 | XY | 194 | GLY |
| 55 | XY | 303 | ARG |
| 55 | XY | 306 | ARG |
| 55 | XY | 323 | ASN |
| 4 | RE | 52 | LEU |
| 42 | QK | 117 | ASN |
| 44 | QM | 12 | ASN |
| 48 | QQ | 68 | ARG |
| 55 | QY | 329 | LEU |
| 55 | XY | 229 | SER |
| 11 | RP | 29 | LYS |
| 23 | R1 | 3 | LYS |
| 55 | QY | 101 | LEU |
| 26 | Y4 | 45 | GLY |
| 52 | XU | 7 | ARG |
| 33 | QB | 127 | ILE |
| 44 | QM | 67 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | QS | 12 | ASP |
| 55 | QY | 323 | ASN |
| 5 | YF | 130 | ALA |
| 11 | YP | 29 | LYS |
| 26 | Y4 | 55 | ARG |
| 38 | XG | 7 | ALA |
| 51 | XT | 100 | ILE |
| 55 | XY | 241 | ASP |
| 55 | XY | 101 | LEU |
| 55 | QY | 162 | ILE |
| 17 | RV | 79 | VAL |
| 41 | QJ | 77 | PRO |
| 55 | QY | 194 | GLY |
| 17 | YV | 79 | VAL |

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 X-ray entries followed by that with respect to entries of similar resolution.

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | RD | 214/218 (98%) | 206 (96%) | 8 (4%) | 41 | 79 |
| 3 | YD | 215/218 (99%) | 210 (98%) | 5 (2%) | 58 | 87 |
| 4 | RE | 164/166 (99%) | 157 (96%) | 7 (4%) | 35 | 75 |
| 4 | YE | 164/166 (99%) | 156 (95%) | 8 (5%) | 31 | 72 |
| 5 | RF | 160/166 (96%) | 151 (94%) | 9 (6%) | 26 | 68 |
| 5 | YF | 159/166 (96%) | 149 (94%) | 10 (6%) | 22 | 63 |
| 6 | RG | 144/156 (92%) | 136 (94%) | 8 (6%) | 26 | 68 |
| 6 | YG | 142/156 (91%) | 131 (92%) | 11 (8%) | 16 | 54 |
| 7 | RH | 144/148 (97%) | 141 (98%) | 3 (2%) | 61 | 88 |
| 7 | YH | 143/148 (97%) | 133 (93%) | 10 (7%) | 19 | 58 |
| 8 | RI | 111/124 (90%) | 102 (92%) | 9 (8%) | 15 | 51 |
| 8 | YI | 108/124 (87%) | 101 (94%) | 7 (6%) | 21 | 61 |
| 9 | RN | 119/119 (100%) | 111 (93%) | 8 (7%) | 20 | 60 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 9 | YN | 118/119 (99%) | 114 (97%) | 4 (3%) | 44 | 80 |
| 10 | RO | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 10 | YO | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 11 | RP | 115/116 (99%) | 113 (98%) | 2 (2%) | 68 | 90 |
| 11 | YP | 115/116 (99%) | 113 (98%) | 2 (2%) | 68 | 90 |
| 12 | RQ | 111/111 (100%) | 108 (97%) | 3 (3%) | 52 | 85 |
| 12 | YQ | 111/111 (100%) | 105 (95%) | 6 (5%) | 27 | 68 |
| 13 | RR | 101/101 (100%) | 95 (94%) | 6 (6%) | 24 | 65 |
| 13 | YR | 101/101 (100%) | 95 (94%) | 6 (6%) | 24 | 65 |
| 14 | RS | 87/88 (99%) | 85 (98%) | 2 (2%) | 58 | 87 |
| 14 | YS | 85/88 (97%) | 83 (98%) | 2 (2%) | 57 | 86 |
| 15 | RT | 115/127 (91%) | 111 (96%) | 4 (4%) | 43 | 80 |
| 15 | YT | 113/127 (89%) | 110 (97%) | 3 (3%) | 52 | 85 |
| 16 | RU | 93/94 (99%) | 89 (96%) | 4 (4%) | 35 | 75 |
| 16 | YU | 93/94 (99%) | 90 (97%) | 3 (3%) | 46 | 81 |
| 17 | RV | 81/82 (99%) | 77 (95%) | 4 (5%) | 31 | 72 |
| 17 | YV | 80/82 (98%) | 76 (95%) | 4 (5%) | 30 | 71 |
| 18 | RW | 90/92 (98%) | 84 (93%) | 6 (7%) | 20 | 60 |
| 18 | YW | 90/92 (98%) | 87 (97%) | 3 (3%) | 45 | 81 |
| 19 | RX | 77/78 (99%) | 76 (99%) | 1 (1%) | 76 | 92 |
| 19 | YX | 77/78 (99%) | 77 (100%) | 0 | 100 | 100 |
| 20 | RY | 86/91 (94%) | 84 (98%) | 2 (2%) | 58 | 87 |
| 20 | YY | 86/91 (94%) | 83 (96%) | 3 (4%) | 43 | 80 |
| 21 | RZ | 159/179 (89%) | 153 (96%) | 6 (4%) | 40 | 78 |
| 21 | YZ | 156/179 (87%) | 150 (96%) | 6 (4%) | 40 | 78 |
| 22 | R0 | 61/67 (91%) | 59 (97%) | 2 (3%) | 45 | 81 |
| 22 | Y0 | 61/67 (91%) | 60 (98%) | 1 (2%) | 70 | 91 |
| 23 | R1 | 79/83 (95%) | 77 (98%) | 2 (2%) | 55 | 86 |
| 23 | Y1 | 81/83 (98%) | 77 (95%) | 4 (5%) | 31 | 72 |
| 24 | R2 | 65/67 (97%) | 63 (97%) | 2 (3%) | 47 | 82 |
| 24 | Y2 | 66/67 (98%) | 64 (97%) | 2 (3%) | 48 | 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 25 | R3 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 25 | Y3 | 50/52 (96%) | 44 (88%) | 6 (12%) | 6 | 28 |
| 26 | R4 | 58/63 (92%) | 56 (97%) | 2 (3%) | 44 | 80 |
| 26 | Y4 | 54/63 (86%) | 46 (85%) | 8 (15%) | 4 | 18 |
| 27 | R5 | 51/52 (98%) | 49 (96%) | 2 (4%) | 39 | 78 |
| 27 | Y5 | 50/52 (96%) | 48 (96%) | 2 (4%) | 38 | 77 |
| 28 | R6 | 51/52 (98%) | 49 (96%) | 2 (4%) | 39 | 78 |
| 28 | Y6 | 50/52 (96%) | 50 (100%) | 0 | 100 | 100 |
| 29 | R7 | 41/42 (98%) | 41 (100%) | 0 | 100 | 100 |
| 29 | Y7 | 41/42 (98%) | 41 (100%) | 0 | 100 | 100 |
| 30 | R8 | 54/55 (98%) | 51 (94%) | 3 (6%) | 26 | 68 |
| 30 | Y8 | 54/55 (98%) | 52 (96%) | 2 (4%) | 41 | 79 |
| 31 | R9 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 31 | Y9 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 33 | QB | 191/220 (87%) | 180 (94%) | 11 (6%) | 25 | 66 |
| 33 | XB | 187/220 (85%) | 173 (92%) | 14 (8%) | 17 | 55 |
| 34 | QC | 144/188 (77%) | 142 (99%) | 2 (1%) | 74 | 92 |
| 34 | XC | 140/188 (74%) | 137 (98%) | 3 (2%) | 61 | 88 |
| 35 | QD | 171/181 (94%) | 166 (97%) | 5 (3%) | 50 | 83 |
| 35 | XD | 172/181 (95%) | 169 (98%) | 3 (2%) | 68 | 90 |
| 36 | QE | 114/123 (93%) | 113 (99%) | 1 (1%) | 84 | 95 |
| 36 | XE | 114/123 (93%) | 113 (99%) | 1 (1%) | 84 | 95 |
| 37 | QF | 85/90 (94%) | 85 (100%) | 0 | 100 | 100 |
| 37 | XF | 85/90 (94%) | 84 (99%) | 1 (1%) | 78 | 93 |
| 38 | QG | 120/127 (94%) | 114 (95%) | 6 (5%) | 30 | 71 |
| 38 | XG | 119/127 (94%) | 115 (97%) | 4 (3%) | 44 | 80 |
| 39 | QH | 116/119 (98%) | 113 (97%) | 3 (3%) | 54 | 85 |
| 39 | XH | 114/119 (96%) | 110 (96%) | 4 (4%) | 43 | 80 |
| 40 | QI | 91/99 (92%) | 83 (91%) | 8 (9%) | 12 | 45 |
| 40 | XI | 88/99 (89%) | 83 (94%) | 5 (6%) | 25 | 67 |
| 41 | QJ | 68/92 (74%) | 66 (97%) | 2 (3%) | 50 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 41 | XJ | 68/92 (74%) | 67 (98%) | 1 (2%) | 72 | 91 |
| 42 | QK | 83/99 (84%) | 81 (98%) | 2 (2%) | 57 | 86 |
| 42 | XK | 83/99 (84%) | 83 (100%) | 0 | 100 | 100 |
| 43 | QL | 96/108 (89%) | 95 (99%) | 1 (1%) | 82 | 95 |
| 43 | XL | 96/108 (89%) | 95 (99%) | 1 (1%) | 82 | 95 |
| 44 | QM | 90/101 (89%) | 87 (97%) | 3 (3%) | 45 | 81 |
| 44 | XM | 87/101 (86%) | 86 (99%) | 1 (1%) | 80 | 94 |
| 45 | QN | 49/50 (98%) | 44 (90%) | 5 (10%) | 9 | 36 |
| 45 | XN | 49/50 (98%) | 48 (98%) | 1 (2%) | 63 | 88 |
| 46 | QO | 78/80 (98%) | 74 (95%) | 4 (5%) | 29 | 70 |
| 46 | XO | 78/80 (98%) | 75 (96%) | 3 (4%) | 40 | 78 |
| 47 | QP | 69/74 (93%) | 68 (99%) | 1 (1%) | 74 | 92 |
| 47 | XP | 68/74 (92%) | 66 (97%) | 2 (3%) | 50 | 83 |
| 48 | QQ | 94/97 (97%) | 94 (100%) | 0 | 100 | 100 |
| 48 | XQ | 94/97 (97%) | 94 (100%) | 0 | 100 | 100 |
| 49 | QR | 59/77 (77%) | 59 (100%) | 0 | 100 | 100 |
| 49 | XR | 59/77 (77%) | 58 (98%) | 1 (2%) | 68 | 90 |
| 50 | QS | 68/80 (85%) | 66 (97%) | 2 (3%) | 50 | 83 |
| 50 | XS | 67/80 (84%) | 67 (100%) | 0 | 100 | 100 |
| 51 | QT | 71/82 (87%) | 68 (96%) | 3 (4%) | 36 | 75 |
| 51 | XT | 70/82 (85%) | 69 (99%) | 1 (1%) | 74 | 92 |
| 52 | QU | 18/22 (82%) | 18 (100%) | 0 | 100 | 100 |
| 52 | XU | 18/22 (82%) | 17 (94%) | 1 (6%) | 26 | 68 |
| 55 | QY | 210/299 (70%) | 200 (95%) | 10 (5%) | 31 | 72 |
| 55 | XY | 211/299 (71%) | 198 (94%) | 13 (6%) | 23 | 64 |
| All | All | 9765/10662 (92%) | 9411 (96%) | 354 (4%) | 42 | 79 |

All (354) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | RD | 88 | ARG |
| 3 | RD | 94 | LEU |
| 3 | RD | 99 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | RD | 111 | LEU |
| 3 | RD | 126 | GLN |
| 3 | RD | 211 | ARG |
| 3 | RD | 242 | ARG |
| 3 | RD | 260 | ARG |
| 4 | RE | 9 | VAL |
| 4 | RE | 82 | ARG |
| 4 | RE | 111 | ARG |
| 4 | RE | 116 | VAL |
| 4 | RE | 119 | ARG |
| 4 | RE | 144 | ARG |
| 4 | RE | 184 | VAL |
| 5 | RF | 33 | LEU |
| 5 | RF | 60 | SER |
| 5 | RF | 74 | ARG |
| 5 | RF | 110 | LEU |
| 5 | RF | 125 | LEU |
| 5 | RF | 168 | ARG |
| 5 | RF | 170 | LEU |
| 5 | RF | 192 | LEU |
| 5 | RF | 205 | ARG |
| 6 | RG | 7 | LEU |
| 6 | RG | 31 | VAL |
| 6 | RG | 53 | LEU |
| 6 | RG | 79 | ASN |
| 6 | RG | 135 | LEU |
| 6 | RG | 146 | TYR |
| 6 | RG | 153 | ARG |
| 6 | RG | 170 | ARG |
| 7 | RH | 6 | ARG |
| 7 | RH | 23 | ARG |
| 7 | RH | 69 | ARG |
| 8 | RI | 10 | GLU |
| 8 | RI | 12 | LEU |
| 8 | RI | 57 | ARG |
| 8 | RI | 60 | GLU |
| 8 | RI | 61 | ARG |
| 8 | RI | 69 | LYS |
| 8 | RI | 75 | LEU |
| 8 | RI | 77 | LEU |
| 8 | RI | 101 | LEU |
| 9 | RN | 7 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | RN | 33 | LEU |
| 9 | RN | 48 | MET |
| 9 | RN | 61 | ARG |
| 9 | RN | 87 | LEU |
| 9 | RN | 99 | LEU |
| 9 | RN | 120 | LEU |
| 9 | RN | 131 | GLN |
| 11 | RP | 112 | LEU |
| 11 | RP | 119 | GLU |
| 12 | RQ | 21 | THR |
| 12 | RQ | 56 | ARG |
| 12 | RQ | 60 | ARG |
| 13 | RR | 18 | LEU |
| 13 | RR | 33 | ARG |
| 13 | RR | 44 | LEU |
| 13 | RR | 54 | LEU |
| 13 | RR | 75 | LEU |
| 13 | RR | 79 | LEU |
| 14 | RS | 43 | GLU |
| 14 | RS | 59 | LYS |
| 15 | RT | 6 | LEU |
| 15 | RT | 35 | LYS |
| 15 | RT | 53 | ARG |
| 15 | RT | 96 | ARG |
| 16 | RU | 5 | LYS |
| 16 | RU | 36 | ARG |
| 16 | RU | 74 | LEU |
| 16 | RU | 92 | ARG |
| 17 | RV | 18 | LEU |
| 17 | RV | 21 | ARG |
| 17 | RV | 62 | LEU |
| 17 | RV | 79 | VAL |
| 18 | RW | 4 | LYS |
| 18 | RW | 11 | ARG |
| 18 | RW | 15 | ARG |
| 18 | RW | 23 | LEU |
| 18 | RW | 51 | LEU |
| 18 | RW | 67 | ASP |
| 19 | RX | 66 | LEU |
| 20 | RY | 23 | ARG |
| 20 | RY | 102 | CYS |
| 21 | RZ | 61 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | RZ | 72 | ARG |
| 21 | RZ | 150 | LEU |
| 21 | RZ | 156 | LYS |
| 21 | RZ | 171 | ILE |
| 21 | RZ | 185 | GLU |
| 22 | R0 | 11 | ARG |
| 22 | R0 | 55 | ARG |
| 23 | R1 | 40 | ARG |
| 23 | R1 | 52 | ARG |
| 24 | R2 | 32 | LEU |
| 24 | R2 | 53 | LEU |
| 26 | R4 | 46 | GLN |
| 26 | R4 | 58 | ARG |
| 27 | R5 | 29 | THR |
| 27 | R5 | 40 | LYS |
| 28 | R6 | 6 | ARG |
| 28 | R6 | 28 | ARG |
| 30 | R8 | 31 | HIS |
| 30 | R8 | 32 | LEU |
| 30 | R8 | 34 | TRP |
| 33 | QB | 15 | VAL |
| 33 | QB | 16 | HIS |
| 33 | QB | 21 | ARG |
| 33 | QB | 24 | TRP |
| 33 | QB | 135 | GLN |
| 33 | QB | 144 | ARG |
| 33 | QB | 157 | ARG |
| 33 | QB | 163 | PHE |
| 33 | QB | 170 | GLU |
| 33 | QB | 187 | LEU |
| 33 | QB | 195 | ASP |
| 34 | QC | 36 | ASP |
| 34 | QC | 131 | ARG |
| 35 | QD | 8 | VAL |
| 35 | QD | 31 | CYS |
| 35 | QD | 49 | ARG |
| 35 | QD | 58 | LEU |
| 35 | QD | 188 | LEU |
| 36 | QE | 41 | VAL |
| 38 | QG | 15 | ASP |
| 38 | QG | 56 | GLN |
| 38 | QG | 57 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | QG | 86 | GLN |
| 38 | QG | 104 | LEU |
| 38 | QG | 114 | ARG |
| 39 | QH | 21 | LYS |
| 39 | QH | 63 | LEU |
| 39 | QH | 84 | ARG |
| 40 | QI | 2 | GLU |
| 40 | QI | 25 | LYS |
| 40 | QI | 42 | ARG |
| 40 | QI | 65 | VAL |
| 40 | QI | 66 | ARG |
| 40 | QI | 92 | TYR |
| 40 | QI | 93 | ARG |
| 40 | QI | 104 | ARG |
| 41 | QJ | 5 | ARG |
| 41 | QJ | 66 | ARG |
| 42 | QK | 48 | ILE |
| 42 | QK | 117 | ASN |
| 43 | QL | 33 | ARG |
| 44 | QM | 3 | ARG |
| 44 | QM | 11 | ARG |
| 44 | QM | 36 | LYS |
| 45 | QN | 3 | ARG |
| 45 | QN | 18 | VAL |
| 45 | QN | 33 | VAL |
| 45 | QN | 41 | ARG |
| 45 | QN | 57 | ARG |
| 46 | QO | 38 | ARG |
| 46 | QO | 39 | LEU |
| 46 | QO | 41 | GLU |
| 46 | QO | 48 | LYS |
| 47 | QP | 5 | ARG |
| 50 | QS | 41 | VAL |
| 50 | QS | 81 | ARG |
| 51 | QT | 10 | LEU |
| 51 | QT | 65 | LYS |
| 51 | QT | 84 | LEU |
| 55 | QY | 94 | GLN |
| 55 | QY | 95 | GLN |
| 55 | QY | 187 | VAL |
| 55 | QY | 193 | GLN |
| 55 | QY | 195 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 55 | QY | 209 | LEU |
| 55 | QY | 257 | CYS |
| 55 | QY | 265 | LYS |
| 55 | QY | 329 | LEU |
| 55 | QY | 336 | LYS |
| 3 | YD | 88 | ARG |
| 3 | YD | 94 | LEU |
| 3 | YD | 211 | ARG |
| 3 | YD | 242 | ARG |
| 3 | YD | 260 | ARG |
| 4 | YE | 73 | GLU |
| 4 | YE | 75 | VAL |
| 4 | YE | 78 | LEU |
| 4 | YE | 82 | ARG |
| 4 | YE | 111 | ARG |
| 4 | YE | 116 | VAL |
| 4 | YE | 119 | ARG |
| 4 | YE | 144 | ARG |
| 5 | YF | 20 | LEU |
| 5 | YF | 33 | LEU |
| 5 | YF | 74 | ARG |
| 5 | YF | 106 | ARG |
| 5 | YF | 110 | LEU |
| 5 | YF | 170 | LEU |
| 5 | YF | 175 | THR |
| 5 | YF | 192 | LEU |
| 5 | YF | 197 | ASP |
| 5 | YF | 205 | ARG |
| 6 | YG | 3 | LEU |
| 6 | YG | 21 | ARG |
| 6 | YG | 31 | VAL |
| 6 | YG | 47 | LYS |
| 6 | YG | 55 | LYS |
| 6 | YG | 98 | ARG |
| 6 | YG | 135 | LEU |
| 6 | YG | 136 | ARG |
| 6 | YG | 146 | TYR |
| 6 | YG | 167 | GLU |
| 6 | YG | 170 | ARG |
| 7 | YH | 3 | ARG |
| 7 | YH | 33 | LEU |
| 7 | YH | 41 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | YH | 46 | GLU |
| 7 | YH | 81 | GLU |
| 7 | YH | 84 | SER |
| 7 | YH | 88 | LEU |
| 7 | YH | 95 | ARG |
| 7 | YH | 140 | LYS |
| 7 | YH | 171 | LEU |
| 8 | YI | 44 | LEU |
| 8 | YI | 50 | ARG |
| 8 | YI | 68 | LEU |
| 8 | YI | 75 | LEU |
| 8 | YI | 77 | LEU |
| 8 | YI | 92 | VAL |
| 8 | YI | 116 | LEU |
| 9 | YN | 48 | MET |
| 9 | YN | 87 | LEU |
| 9 | YN | 99 | LEU |
| 9 | YN | 131 | GLN |
| 11 | YP | 70 | GLN |
| 11 | YP | 112 | LEU |
| 12 | YQ | 7 | MET |
| 12 | YQ | 21 | THR |
| 12 | YQ | 56 | ARG |
| 12 | YQ | 60 | ARG |
| 12 | YQ | 79 | LEU |
| 12 | YQ | 109 | VAL |
| 13 | YR | 28 | LEU |
| 13 | YR | 44 | LEU |
| 13 | YR | 65 | LEU |
| 13 | YR | 75 | LEU |
| 13 | YR | 79 | LEU |
| 13 | YR | 100 | LEU |
| 14 | YS | 20 | ARG |
| 14 | YS | 67 | ARG |
| 15 | YT | 23 | ARG |
| 15 | YT | 53 | ARG |
| 15 | YT | 96 | ARG |
| 16 | YU | 36 | ARG |
| 16 | YU | 74 | LEU |
| 16 | YU | 89 | GLU |
| 17 | YV | 6 | LYS |
| 17 | YV | 18 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | YV | 53 | GLU |
| 17 | YV | 62 | LEU |
| 18 | YW | 11 | ARG |
| 18 | YW | 23 | LEU |
| 18 | YW | 67 | ASP |
| 20 | YY | 6 | HIS |
| 20 | YY | 23 | ARG |
| 20 | YY | 102 | CYS |
| 21 | YZ | 6 | LYS |
| 21 | YZ | 46 | LYS |
| 21 | YZ | 72 | ARG |
| 21 | YZ | 91 | LEU |
| 21 | YZ | 150 | LEU |
| 21 | YZ | 156 | LYS |
| 22 | Y0 | 35 | ASN |
| 23 | Y1 | 21 | ARG |
| 23 | Y1 | 40 | ARG |
| 23 | Y1 | 52 | ARG |
| 23 | Y1 | 85 | LEU |
| 24 | Y2 | 32 | LEU |
| 24 | Y2 | 53 | LEU |
| 25 | Y3 | 3 | ARG |
| 25 | Y3 | 23 | LEU |
| 25 | Y3 | 30 | ARG |
| 25 | Y3 | 44 | ARG |
| 25 | Y3 | 54 | VAL |
| 25 | Y3 | 55 | ARG |
| 26 | Y4 | 46 | GLN |
| 26 | Y4 | 48 | ARG |
| 26 | Y4 | 58 | ARG |
| 26 | Y4 | 60 | GLN |
| 26 | Y4 | 61 | ARG |
| 26 | Y4 | 62 | ARG |
| 26 | Y4 | 67 | TYR |
| 26 | Y4 | 69 | LYS |
| 27 | Y5 | 29 | THR |
| 27 | Y5 | 40 | LYS |
| 30 | Y8 | 31 | HIS |
| 30 | Y8 | 34 | TRP |
| 33 | XB | 8 | LYS |
| 33 | XB | 24 | TRP |
| 33 | XB | 76 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | XB | 118 | LEU |
| 33 | XB | 122 | PHE |
| 33 | XB | 127 | ILE |
| 33 | XB | 158 | LEU |
| 33 | XB | 163 | PHE |
| 33 | XB | 170 | GLU |
| 33 | XB | 187 | LEU |
| 33 | XB | 195 | ASP |
| 33 | XB | 212 | GLN |
| 33 | XB | 217 | ARG |
| 33 | XB | 224 | GLN |
| 34 | XC | 21 | ARG |
| 34 | XC | 105 | GLU |
| 34 | XC | 190 | ARG |
| 35 | XD | 8 | VAL |
| 35 | XD | 31 | CYS |
| 35 | XD | 122 | ARG |
| 36 | XE | 41 | VAL |
| 37 | XF | 28 | ARG |
| 38 | XG | 15 | ASP |
| 38 | XG | 78 | ARG |
| 38 | XG | 114 | ARG |
| 38 | XG | 115 | ARG |
| 39 | XH | 21 | LYS |
| 39 | XH | 63 | LEU |
| 39 | XH | 98 | LYS |
| 39 | XH | 112 | LEU |
| 40 | XI | 23 | ASN |
| 40 | XI | 65 | VAL |
| 40 | XI | 92 | TYR |
| 40 | XI | 102 | LEU |
| 40 | XI | 104 | ARG |
| 41 | XJ | 57 | LYS |
| 43 | XL | 41 | ARG |
| 44 | XM | 70 | LEU |
| 45 | XN | 57 | ARG |
| 46 | XO | 38 | ARG |
| 46 | XO | 39 | LEU |
| 46 | XO | 68 | ARG |
| 47 | XP | 8 | ARG |
| 47 | XP | 28 | ARG |
| 49 | XR | 58 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | XT | 84 | LEU |
| 52 | XU | 10 | ARG |
| 55 | XY | 107 | ASP |
| 55 | XY | 153 | GLU |
| 55 | XY | 187 | VAL |
| 55 | XY | 193 | GLN |
| 55 | XY | 274 | LEU |
| 55 | XY | 305 | ASP |
| 55 | XY | 306 | ARG |
| 55 | XY | 311 | ASN |
| 55 | XY | 318 | THR |
| 55 | XY | 325 | THR |
| 55 | XY | 326 | LEU |
| 55 | XY | 329 | LEU |
| 55 | XY | 336 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | RP | 9 | ASN |
| 31 | R9 | 20 | HIS |
| 9 | YN | 131 | GLN |
| 34 | XC | 6 | HIS |
| 40 | XI | 124 | GLN |
| 50 | XS | 23 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | RA | 2855/2915 (97%) | 442 (15%) | 27 (0%) |
| 1 | YA | 2855/2915 (97%) | 439 (15%) | 25 (0%) |
| 2 | RB | 119/122 (97%) | 9 (7%) | 0 |
| 2 | YB | 119/122 (97%) | 10 (8%) | 0 |
| 32 | QA | 1494/1521 (98%) | 229 (15%) | 16 (1%) |
| 32 | XA | 1498/1521 (98%) | 227 (15%) | 19 (1%) |
| 53 | QV | 76/77 (98%) | 15 (19%) | 0 |
| 53 | XV | 76/77 (98%) | 15 (19%) | 1 (1%) |
| 54 | QX | 9/25 (36%) | 2 (22%) | 0 |
| 54 | XX | 8/25 (32%) | 3 (37%) | 0 |
| All | All | 9109/9320 (97%) | 1391 (15%) | 88 (0%) |

All (1391) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | RA | 10 | G |
| 1 | RA | 11 | G |
| 1 | RA | 12 | U |
| 1 | RA | 15 | G |
| 1 | RA | 45 | C |
| 1 | RA | 71 | A |
| 1 | RA | 74 | A |
| 1 | RA | 75 | G |
| 1 | RA | 84 | A |
| 1 | RA | 92 | A |
| 1 | RA | 95 | G |
| 1 | RA | 102 | G |
| 1 | RA | 118 | A |
| 1 | RA | 119 | A |
| 1 | RA | 120 | U |
| 1 | RA | 131 | G |
| 1 | RA | 141 | A |
| 1 | RA | 157 | U |
| 1 | RA | 196 | A |
| 1 | RA | 199 | A |
| 1 | RA | 205 | G |
| 1 | RA | 215 | G |
| 1 | RA | 216 | A |
| 1 | RA | 221 | A |
| 1 | RA | 222 | A |
| 1 | RA | 229 | A |
| 1 | RA | 230 | U |
| 1 | RA | 248 | G |
| 1 | RA | 272(K) | U |
| 1 | RA | 272(L) | U |
| 1 | RA | 272(M) | G |
| 1 | RA | 272(N) | U |
| 1 | RA | 272(O) | C |
| 1 | RA | 273(B) | U |
| 1 | RA | 273(C) | G |
| 1 | RA | 273(K) | C |
| 1 | RA | 277 | C |
| 1 | RA | 278 | A |
| 1 | RA | 279 | C |
| 1 | RA | 311 | A |
| 1 | RA | 317 | G |
| 1 | RA | 324 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | RA | 327 | G |
| 1 | RA | 329 | G |
| 1 | RA | 330 | A |
| 1 | RA | 342 | G |
| 1 | RA | 352 | G |
| 1 | RA | 362 | U |
| 1 | RA | 363(A) | G |
| 1 | RA | 372 | G |
| 1 | RA | 386 | G |
| 1 | RA | 396 | G |
| 1 | RA | 405 | U |
| 1 | RA | 411 | G |
| 1 | RA | 412 | A |
| 1 | RA | 428 | A |
| 1 | RA | 444 | C |
| 1 | RA | 455 | C |
| 1 | RA | 456 | C |
| 1 | RA | 457 | A |
| 1 | RA | 470 | A |
| 1 | RA | 481 | G |
| 1 | RA | 505 | A |
| 1 | RA | 509 | C |
| 1 | RA | 530 | G |
| 1 | RA | 531 | C |
| 1 | RA | 532 | A |
| 1 | RA | 533 | G |
| 1 | RA | 545 | G |
| 1 | RA | 563 | G |
| 1 | RA | 573 | G |
| 1 | RA | 575 | A |
| 1 | RA | 586 | A |
| 1 | RA | 603 | A |
| 1 | RA | 604 | G |
| 1 | RA | 607 | U |
| 1 | RA | 610 | G |
| 1 | RA | 615 | G |
| 1 | RA | 627 | A |
| 1 | RA | 634 | C |
| 1 | RA | 637 | A |
| 1 | RA | 645 | C |
| 1 | RA | 646 | A |
| 1 | RA | 652(C) | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | RA | 652(D) | G |
| 1 | RA | 652(V) | G |
| 1 | RA | 653 | A |
| 1 | RA | 669 | G |
| 1 | RA | 686 | G |
| 1 | RA | 715 | G |
| 1 | RA | 717 | G |
| 1 | RA | 730 | C |
| 1 | RA | 752 | A |
| 1 | RA | 753 | C |
| 1 | RA | 764 | A |
| 1 | RA | 775 | G |
| 1 | RA | 776 | G |
| 1 | RA | 782 | A |
| 1 | RA | 784 | A |
| 1 | RA | 785 | G |
| 1 | RA | 792 | G |
| 1 | RA | 805 | G |
| 1 | RA | 812 | C |
| 1 | RA | 827 | U |
| 1 | RA | 828 | U |
| 1 | RA | 857 | C |
| 1 | RA | 859 | G |
| 1 | RA | 877 | U |
| 1 | RA | 880 | G |
| 1 | RA | 886 | C |
| 1 | RA | 887 | A |
| 1 | RA | 888 | C |
| 1 | RA | 889 | C |
| 1 | RA | 890 | A |
| 1 | RA | 893 | C |
| 1 | RA | 896 | A |
| 1 | RA | 900 | A |
| 1 | RA | 901 | A |
| 1 | RA | 907 | U |
| 1 | RA | 910 | A |
| 1 | RA | 915 | C |
| 1 | RA | 917 | A |
| 1 | RA | 931 | G |
| 1 | RA | 932 | G |
| 1 | RA | 941 | A |
| 1 | RA | 945 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | RA | 946 | G |
| 1 | RA | 953 | A |
| 1 | RA | 959 | A |
| 1 | RA | 961 | C |
| 1 | RA | 974 | G |
| 1 | RA | 975(A) | C |
| 1 | RA | 980 | A |
| 1 | RA | 983 | A |
| 1 | RA | 996 | A |
| 1 | RA | 1012 | U |
| 1 | RA | 1013 | C |
| 1 | RA | 1017 | G |
| 1 | RA | 1025 | G |
| 1 | RA | 1033 | U |
| 1 | RA | 1038 | C |
| 1 | RA | 1044 | G |
| 1 | RA | 1046 | A |
| 1 | RA | 1047 | G |
| 1 | RA | 1048 | A |
| 1 | RA | 1052 | C |
| 1 | RA | 1053 | C |
| 1 | RA | 1054 | A |
| 1 | RA | 1058 | G |
| 1 | RA | 1060 | U |
| 1 | RA | 1063 | G |
| 1 | RA | 1064 | C |
| 1 | RA | 1065 | U |
| 1 | RA | 1066 | U |
| 1 | RA | 1067 | A |
| 1 | RA | 1068 | G |
| 1 | RA | 1069 | A |
| 1 | RA | 1070 | A |
| 1 | RA | 1071 | G |
| 1 | RA | 1072 | C |
| 1 | RA | 1073 | A |
| 1 | RA | 1074 | G |
| 1 | RA | 1076 | C |
| 1 | RA | 1077 | A |
| 1 | RA | 1078 | U |
| 1 | RA | 1079 | C |
| 1 | RA | 1082 | U |
| 1 | RA | 1083 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | RA | 1084 | A |
| 1 | RA | 1085 | A |
| 1 | RA | 1086 | A |
| 1 | RA | 1088 | A |
| 1 | RA | 1090 | U |
| 1 | RA | 1091 | G |
| 1 | RA | 1092 | C |
| 1 | RA | 1094 | U |
| 1 | RA | 1096 | A |
| 1 | RA | 1098 | A |
| 1 | RA | 1109 | C |
| 1 | RA | 1110 | G |
| 1 | RA | 1111 | A |
| 1 | RA | 1112 | G |
| 1 | RA | 1126 | A |
| 1 | RA | 1130 | U |
| 1 | RA | 1135 | C |
| 1 | RA | 1136 | G |
| 1 | RA | 1142(B) | A |
| 1 | RA | 1171 | G |
| 1 | RA | 1206 | G |
| 1 | RA | 1211 | U |
| 1 | RA | 1212 | G |
| 1 | RA | 1220 | A |
| 1 | RA | 1236 | G |
| 1 | RA | 1253 | A |
| 1 | RA | 1256 | G |
| 1 | RA | 1271 | G |
| 1 | RA | 1272 | A |
| 1 | RA | 1273 | U |
| 1 | RA | 1300 | U |
| 1 | RA | 1301 | A |
| 1 | RA | 1314 | C |
| 1 | RA | 1352 | U |
| 1 | RA | 1359 | A |
| 1 | RA | 1360 | A |
| 1 | RA | 1365 | A |
| 1 | RA | 1368 | G |
| 1 | RA | 1380 | G |
| 1 | RA | 1384 | A |
| 1 | RA | 1385 | G |
| 1 | RA | 1416 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | RA | 1417 | C |
| 1 | RA | 1420 | U |
| 1 | RA | 1421 | G |
| 1 | RA | 1428 | C |
| 1 | RA | 1445(A) | A |
| 1 | RA | 1450(A) | G |
| 1 | RA | 1455 | G |
| 1 | RA | 1459 | G |
| 1 | RA | 1467 | C |
| 1 | RA | 1471 | A |
| 1 | RA | 1482 | G |
| 1 | RA | 1493 | C |
| 1 | RA | 1494 | A |
| 1 | RA | 1497 | U |
| 1 | RA | 1508 | A |
| 1 | RA | 1509(A) | C |
| 1 | RA | 1509(B) | A |
| 1 | RA | 1531 | C |
| 1 | RA | 1542 | A |
| 1 | RA | 1543 | C |
| 1 | RA | 1547 | C |
| 1 | RA | 1558 | A |
| 1 | RA | 1559 | G |
| 1 | RA | 1566 | A |
| 1 | RA | 1569 | A |
| 1 | RA | 1578 | U |
| 1 | RA | 1580 | A |
| 1 | RA | 1584 | C |
| 1 | RA | 1586 | A |
| 1 | RA | 1608 | A |
| 1 | RA | 1609 | A |
| 1 | RA | 1610 | A |
| 1 | RA | 1640 | C |
| 1 | RA | 1648 | C |
| 1 | RA | 1674 | G |
| 1 | RA | 1696 | G |
| 1 | RA | 1700 | A |
| 1 | RA | 1701 | A |
| 1 | RA | 1721 | G |
| 1 | RA | 1722 | A |
| 1 | RA | 1740 | G |
| 1 | RA | 1750 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | RA | 1756 | G |
| 1 | RA | 1762 | A |
| 1 | RA | 1763 | G |
| 1 | RA | 1764 | G |
| 1 | RA | 1773 | A |
| 1 | RA | 1780 | A |
| 1 | RA | 1786 | A |
| 1 | RA | 1791 | A |
| 1 | RA | 1800 | C |
| 1 | RA | 1801 | G |
| 1 | RA | 1812 | A |
| 1 | RA | 1816 | G |
| 1 | RA | 1835 | G |
| 1 | RA | 1847 | A |
| 1 | RA | 1848 | A |
| 1 | RA | 1877 | A |
| 1 | RA | 1878 | G |
| 1 | RA | 1900 | A |
| 1 | RA | 1906 | G |
| 1 | RA | 1914 | C |
| 1 | RA | 1915 | 5MU |
| 1 | RA | 1927 | A |
| 1 | RA | 1929 | G |
| 1 | RA | 1930 | G |
| 1 | RA | 1936 | A |
| 1 | RA | 1938 | A |
| 1 | RA | 1955 | U |
| 1 | RA | 1963 | U |
| 1 | RA | 1967 | C |
| 1 | RA | 1970 | A |
| 1 | RA | 1971 | A |
| 1 | RA | 1972 | A |
| 1 | RA | 1975 | G |
| 1 | RA | 1993 | U |
| 1 | RA | 1997 | G |
| 1 | RA | 2023 | G |
| 1 | RA | 2031 | A |
| 1 | RA | 2032 | G |
| 1 | RA | 2033 | A |
| 1 | RA | 2043 | C |
| 1 | RA | 2055 | C |
| 1 | RA | 2056 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | RA | 2060 | A |
| 1 | RA | 2061 | G |
| 1 | RA | 2062 | A |
| 1 | RA | 2069 | G |
| 1 | RA | 2096 | U |
| 1 | RA | 2099 | U |
| 1 | RA | 2103 | C |
| 1 | RA | 2105 | C |
| 1 | RA | 2107 | C |
| 1 | RA | 2108 | C |
| 1 | RA | 2109 | U |
| 1 | RA | 2112 | G |
| 1 | RA | 2115 | G |
| 1 | RA | 2116 | G |
| 1 | RA | 2117 | A |
| 1 | RA | 2118 | U |
| 1 | RA | 2119 | A |
| 1 | RA | 2121 | G |
| 1 | RA | 2123 | G |
| 1 | RA | 2127 | G |
| 1 | RA | 2129 | C |
| 1 | RA | 2131 | G |
| 1 | RA | 2132 | U |
| 1 | RA | 2133 | G |
| 1 | RA | 2134 | A |
| 1 | RA | 2136 | C |
| 1 | RA | 2138 | C |
| 1 | RA | 2145 | C |
| 1 | RA | 2146 | C |
| 1 | RA | 2147 | G |
| 1 | RA | 2148 | G |
| 1 | RA | 2151 | G |
| 1 | RA | 2158 | A |
| 1 | RA | 2159 | G |
| 1 | RA | 2161 | C |
| 1 | RA | 2163 | C |
| 1 | RA | 2165 | G |
| 1 | RA | 2172 | U |
| 1 | RA | 2173 | A |
| 1 | RA | 2180 | U |
| 1 | RA | 2186 | G |
| 1 | RA | 2189 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | RA | 2192 | G |
| 1 | RA | 2198 | A |
| 1 | RA | 2206 | G |
| 1 | RA | 2207 | G |
| 1 | RA | 2208 | A |
| 1 | RA | 2218 | U |
| 1 | RA | 2225 | A |
| 1 | RA | 2238 | G |
| 1 | RA | 2239 | G |
| 1 | RA | 2269 | A |
| 1 | RA | 2275 | C |
| 1 | RA | 2278 | A |
| 1 | RA | 2283 | C |
| 1 | RA | 2287 | A |
| 1 | RA | 2289 | G |
| 1 | RA | 2291 | U |
| 1 | RA | 2305 | A |
| 1 | RA | 2308 | G |
| 1 | RA | 2311 | A |
| 1 | RA | 2312 | U |
| 1 | RA | 2320 | A |
| 1 | RA | 2321 | G |
| 1 | RA | 2322 | A |
| 1 | RA | 2325 | G |
| 1 | RA | 2334 | G |
| 1 | RA | 2335 | A |
| 1 | RA | 2343 | C |
| 1 | RA | 2347 | C |
| 1 | RA | 2350 | C |
| 1 | RA | 2372 | G |
| 1 | RA | 2379 | G |
| 1 | RA | 2383 | G |
| 1 | RA | 2385 | C |
| 1 | RA | 2406 | U |
| 1 | RA | 2410 | G |
| 1 | RA | 2422 | A |
| 1 | RA | 2424 | C |
| 1 | RA | 2425 | A |
| 1 | RA | 2429 | G |
| 1 | RA | 2430 | A |
| 1 | RA | 2434 | A |
| 1 | RA | 2435 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | RA | 2439 | A |
| 1 | RA | 2441 | C |
| 1 | RA | 2448 | A |
| 1 | RA | 2465 | C |
| 1 | RA | 2466 | C |
| 1 | RA | 2474 | C |
| 1 | RA | 2476 | A |
| 1 | RA | 2478 | A |
| 1 | RA | 2502 | G |
| 1 | RA | 2504 | U |
| 1 | RA | 2505 | G |
| 1 | RA | 2506 | U |
| 1 | RA | 2518 | A |
| 1 | RA | 2527 | C |
| 1 | RA | 2529 | G |
| 1 | RA | 2554 | U |
| 1 | RA | 2555 | U |
| 1 | RA | 2566 | A |
| 1 | RA | 2567 | G |
| 1 | RA | 2573 | C |
| 1 | RA | 2574 | G |
| 1 | RA | 2602 | A |
| 1 | RA | 2603 | G |
| 1 | RA | 2609 | U |
| 1 | RA | 2611 | U |
| 1 | RA | 2612 | C |
| 1 | RA | 2615 | U |
| 1 | RA | 2629 | A |
| 1 | RA | 2630 | G |
| 1 | RA | 2654 | A |
| 1 | RA | 2663 | G |
| 1 | RA | 2689 | U |
| 1 | RA | 2690 | C |
| 1 | RA | 2703 | C |
| 1 | RA | 2712(B) | A |
| 1 | RA | 2713 | A |
| 1 | RA | 2714 | G |
| 1 | RA | 2726 | U |
| 1 | RA | 2732 | G |
| 1 | RA | 2733 | A |
| 1 | RA | 2744 | G |
| 1 | RA | 2751 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | RA | 2757 | A |
| 1 | RA | 2758 | A |
| 1 | RA | 2759 | G |
| 1 | RA | 2764 | A |
| 1 | RA | 2765 | A |
| 1 | RA | 2766 | G |
| 1 | RA | 2769 | C |
| 1 | RA | 2778 | A |
| 1 | RA | 2780 | G |
| 1 | RA | 2811 | G |
| 1 | RA | 2818 | G |
| 1 | RA | 2820 | A |
| 1 | RA | 2821 | A |
| 1 | RA | 2833 | G |
| 1 | RA | 2849 | U |
| 1 | RA | 2872 | G |
| 1 | RA | 2873 | A |
| 1 | RA | 2880 | C |
| 1 | RA | 2886 | G |
| 1 | RA | 2892 | A |
| 1 | RA | 2894 | G |
| 1 | RA | 2897 | U |
| 2 | RB | 2 | C |
| 2 | RB | 9 | G |
| 2 | RB | 13 | A |
| 2 | RB | 30 | C |
| 2 | RB | 56 | G |
| 2 | RB | 73 | A |
| 2 | RB | 84 | C |
| 2 | RB | 106 | G |
| 2 | RB | 110 | G |
| 32 | QA | 5 | U |
| 32 | QA | 7 | G |
| 32 | QA | 9 | G |
| 32 | QA | 32 | A |
| 32 | QA | 39 | G |
| 32 | QA | 47 | C |
| 32 | QA | 48 | C |
| 32 | QA | 50 | A |
| 32 | QA | 51 | A |
| 32 | QA | 61 | G |
| 32 | QA | 79 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 32 | QA | 101 | A |
| 32 | QA | 116 | A |
| 32 | QA | 121 | C |
| 32 | QA | 131 | C |
| 32 | QA | 163 | C |
| 32 | QA | 174 | C |
| 32 | QA | 182 | U |
| 32 | QA | 189(F) | U |
| 32 | QA | 195 | A |
| 32 | QA | 197 | A |
| 32 | QA | 202 | U |
| 32 | QA | 203 | U |
| 32 | QA | 204 | U |
| 32 | QA | 216 | G |
| 32 | QA | 247 | G |
| 32 | QA | 251 | G |
| 32 | QA | 266 | G |
| 32 | QA | 267 | C |
| 32 | QA | 289 | G |
| 32 | QA | 318 | G |
| 32 | QA | 321 | A |
| 32 | QA | 328 | C |
| 32 | QA | 332 | G |
| 32 | QA | 345 | C |
| 32 | QA | 347 | G |
| 32 | QA | 348 | G |
| 32 | QA | 352 | C |
| 32 | QA | 353 | A |
| 32 | QA | 354 | G |
| 32 | QA | 367 | U |
| 32 | QA | 372 | C |
| 32 | QA | 373 | A |
| 32 | QA | 384 | G |
| 32 | QA | 397 | A |
| 32 | QA | 398 | C |
| 32 | QA | 406 | G |
| 32 | QA | 412 | A |
| 32 | QA | 413 | G |
| 32 | QA | 423 | G |
| 32 | QA | 424 | G |
| 32 | QA | 429 | U |
| 32 | QA | 439 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | QA | 442 | C |
| 32 | QA | 452 | A |
| 32 | QA | 458 | C |
| 32 | QA | 461 | A |
| 32 | QA | 470 | C |
| 32 | QA | 485 | G |
| 32 | QA | 496 | A |
| 32 | QA | 498 | U |
| 32 | QA | 505 | G |
| 32 | QA | 509 | A |
| 32 | QA | 510 | A |
| 32 | QA | 511 | C |
| 32 | QA | 518 | C |
| 32 | QA | 521 | G |
| 32 | QA | 527 | 7MG |
| 32 | QA | 532 | A |
| 32 | QA | 547 | A |
| 32 | QA | 559 | A |
| 32 | QA | 561 | U |
| 32 | QA | 564 | C |
| 32 | QA | 572 | A |
| 32 | QA | 573 | A |
| 32 | QA | 575 | G |
| 32 | QA | 576 | G |
| 32 | QA | 577 | G |
| 32 | QA | 592 | G |
| 32 | QA | 596 | C |
| 32 | QA | 619 | U |
| 32 | QA | 630 | G |
| 32 | QA | 631 | G |
| 32 | QA | 632 | A |
| 32 | QA | 653 | A |
| 32 | QA | 661 | G |
| 32 | QA | 665 | A |
| 32 | QA | 687 | A |
| 32 | QA | 688 | G |
| 32 | QA | 695 | A |
| 32 | QA | 721 | G |
| 32 | QA | 723 | U |
| 32 | QA | 731 | G |
| 32 | QA | 753 | A |
| 32 | QA | 755 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | QA | 774 | G |
| 32 | QA | 777 | A |
| 32 | QA | 787 | A |
| 32 | QA | 792 | A |
| 32 | QA | 793 | U |
| 32 | QA | 794 | A |
| 32 | QA | 817 | C |
| 32 | QA | 818 | G |
| 32 | QA | 821 | G |
| 32 | QA | 828 | A |
| 32 | QA | 829 | G |
| 32 | QA | 838 | G |
| 32 | QA | 839 | U |
| 32 | QA | 840 | C |
| 32 | QA | 841 | U |
| 32 | QA | 848 | C |
| 32 | QA | 851 | G |
| 32 | QA | 902 | G |
| 32 | QA | 914 | A |
| 32 | QA | 926 | G |
| 32 | QA | 927 | G |
| 32 | QA | 931 | C |
| 32 | QA | 934 | C |
| 32 | QA | 942 | G |
| 32 | QA | 960 | U |
| 32 | QA | 961 | U |
| 32 | QA | 968 | A |
| 32 | QA | 969 | A |
| 32 | QA | 971 | G |
| 32 | QA | 972 | C |
| 32 | QA | 974 | A |
| 32 | QA | 975 | A |
| 32 | QA | 976 | G |
| 32 | QA | 977 | A |
| 32 | QA | 992 | U |
| 32 | QA | 993 | G |
| 32 | QA | 994 | A |
| 32 | QA | 998 | G |
| 32 | QA | 1002 | G |
| 32 | QA | 1003 | G |
| 32 | QA | 1006 | C |
| 32 | QA | 1009 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | QA | 1020 | U |
| 32 | QA | 1022 | G |
| 32 | QA | 1023 | G |
| 32 | QA | 1024 | G |
| 32 | QA | 1025 | U |
| 32 | QA | 1026 | G |
| 32 | QA | 1027 | C |
| 32 | QA | 1028 | C |
| 32 | QA | 1029 | C |
| 32 | QA | 1030(B) | G |
| 32 | QA | 1030(C) | C |
| 32 | QA | 1030(E) | A |
| 32 | QA | 1032 | G |
| 32 | QA | 1033 | G |
| 32 | QA | 1037 | C |
| 32 | QA | 1042 | G |
| 32 | QA | 1044 | A |
| 32 | QA | 1054 | C |
| 32 | QA | 1065 | U |
| 32 | QA | 1066 | C |
| 32 | QA | 1068 | G |
| 32 | QA | 1081 | G |
| 32 | QA | 1094 | G |
| 32 | QA | 1095 | U |
| 32 | QA | 1101 | A |
| 32 | QA | 1125 | U |
| 32 | QA | 1130 | A |
| 32 | QA | 1134 | G |
| 32 | QA | 1136 | U |
| 32 | QA | 1139 | G |
| 32 | QA | 1140 | C |
| 32 | QA | 1152 | A |
| 32 | QA | 1158 | C |
| 32 | QA | 1159 | U |
| 32 | QA | 1166 | G |
| 32 | QA | 1183 | A |
| 32 | QA | 1184 | G |
| 32 | QA | 1196 | U |
| 32 | QA | 1197 | G |
| 32 | QA | 1202 | G |
| 32 | QA | 1208 | C |
| 32 | QA | 1213 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | QA | 1224 | G |
| 32 | QA | 1227 | A |
| 32 | QA | 1238 | A |
| 32 | QA | 1250 | A |
| 32 | QA | 1256 | A |
| 32 | QA | 1257 | U |
| 32 | QA | 1258 | G |
| 32 | QA | 1270 | C |
| 32 | QA | 1278 | U |
| 32 | QA | 1280 | A |
| 32 | QA | 1281 | U |
| 32 | QA | 1286 | A |
| 32 | QA | 1287 | A |
| 32 | QA | 1299 | A |
| 32 | QA | 1300 | G |
| 32 | QA | 1302 | U |
| 32 | QA | 1305 | G |
| 32 | QA | 1312 | G |
| 32 | QA | 1320 | C |
| 32 | QA | 1338 | G |
| 32 | QA | 1340 | A |
| 32 | QA | 1347 | G |
| 32 | QA | 1353 | G |
| 32 | QA | 1363(A) | C |
| 32 | QA | 1364 | U |
| 32 | QA | 1370 | G |
| 32 | QA | 1394 | A |
| 32 | QA | 1397 | C |
| 32 | QA | 1399 | C |
| 32 | QA | 1401 | G |
| 32 | QA | 1419 | G |
| 32 | QA | 1442(A) | G |
| 32 | QA | 1442(B) | G |
| 32 | QA | 1446 | U |
| 32 | QA | 1447 | A |
| 32 | QA | 1452 | C |
| 32 | QA | 1487 | G |
| 32 | QA | 1492 | A |
| 32 | QA | 1493 | A |
| 32 | QA | 1497 | G |
| 32 | QA | 1499 | A |
| 32 | QA | 1503 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 32 | QA | 1504 | G |
| 32 | QA | 1506 | U |
| 32 | QA | 1517 | G |
| 32 | QA | 1520 | G |
| 32 | QA | 1525 | G |
| 32 | QA | 1529 | G |
| 32 | QA | 1530 | G |
| 32 | QA | 1531 | A |
| 53 | QV | 2 | G |
| 53 | QV | 4 | G |
| 53 | QV | 5 | G |
| 53 | QV | 9 | G |
| 53 | QV | 17(A) | U |
| 53 | QV | 18 | G |
| 53 | QV | 19 | G |
| 53 | QV | 21 | A |
| 53 | QV | 31 | G |
| 53 | QV | 47 | U |
| 53 | QV | 48 | C |
| 53 | QV | 52 | G |
| 53 | QV | 53 | G |
| 53 | QV | 54 | U |
| 53 | QV | 76 | A |
| 54 | QX | 21 | A |
| 54 | QX | 22 | C |
| 1 | YA | 10 | G |
| 1 | YA | 11 | G |
| 1 | YA | 12 | U |
| 1 | YA | 15 | G |
| 1 | YA | 45 | C |
| 1 | YA | 71 | A |
| 1 | YA | 74 | A |
| 1 | YA | 75 | G |
| 1 | YA | 84 | A |
| 1 | YA | 92 | A |
| 1 | YA | 95 | G |
| 1 | YA | 102 | G |
| 1 | YA | 118 | A |
| 1 | YA | 119 | A |
| 1 | YA | 120 | U |
| 1 | YA | 131 | G |
| 1 | YA | 141 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | YA | 157 | U |
| 1 | YA | 196 | A |
| 1 | YA | 199 | A |
| 1 | YA | 205 | G |
| 1 | YA | 215 | G |
| 1 | YA | 216 | A |
| 1 | YA | 221 | A |
| 1 | YA | 222 | A |
| 1 | YA | 229 | A |
| 1 | YA | 230 | U |
| 1 | YA | 248 | G |
| 1 | YA | 272(K) | U |
| 1 | YA | 272(L) | U |
| 1 | YA | 272(M) | G |
| 1 | YA | 272(N) | U |
| 1 | YA | 272(O) | C |
| 1 | YA | 273(B) | U |
| 1 | YA | 273(C) | G |
| 1 | YA | 273(K) | C |
| 1 | YA | 277 | C |
| 1 | YA | 278 | A |
| 1 | YA | 279 | C |
| 1 | YA | 311 | A |
| 1 | YA | 317 | G |
| 1 | YA | 324 | A |
| 1 | YA | 327 | G |
| 1 | YA | 329 | G |
| 1 | YA | 330 | A |
| 1 | YA | 342 | G |
| 1 | YA | 352 | G |
| 1 | YA | 362 | U |
| 1 | YA | 363(A) | G |
| 1 | YA | 372 | G |
| 1 | YA | 386 | G |
| 1 | YA | 396 | G |
| 1 | YA | 405 | U |
| 1 | YA | 411 | G |
| 1 | YA | 412 | A |
| 1 | YA | 428 | A |
| 1 | YA | 444 | C |
| 1 | YA | 455 | C |
| 1 | YA | 456 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | YA | 457 | A |
| 1 | YA | 470 | A |
| 1 | YA | 481 | G |
| 1 | YA | 505 | A |
| 1 | YA | 509 | C |
| 1 | YA | 530 | G |
| 1 | YA | 531 | C |
| 1 | YA | 532 | A |
| 1 | YA | 533 | G |
| 1 | YA | 545 | G |
| 1 | YA | 563 | G |
| 1 | YA | 573 | G |
| 1 | YA | 575 | A |
| 1 | YA | 586 | A |
| 1 | YA | 603 | A |
| 1 | YA | 604 | G |
| 1 | YA | 607 | U |
| 1 | YA | 610 | G |
| 1 | YA | 615 | G |
| 1 | YA | 627 | A |
| 1 | YA | 634 | C |
| 1 | YA | 637 | A |
| 1 | YA | 645 | C |
| 1 | YA | 646 | A |
| 1 | YA | 652(C) | A |
| 1 | YA | 652(D) | G |
| 1 | YA | 652(V) | G |
| 1 | YA | 653 | A |
| 1 | YA | 669 | G |
| 1 | YA | 686 | G |
| 1 | YA | 715 | G |
| 1 | YA | 717 | G |
| 1 | YA | 730 | C |
| 1 | YA | 752 | A |
| 1 | YA | 753 | C |
| 1 | YA | 764 | A |
| 1 | YA | 775 | G |
| 1 | YA | 776 | G |
| 1 | YA | 782 | A |
| 1 | YA | 784 | A |
| 1 | YA | 785 | G |
| 1 | YA | 792 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | YA | 805 | G |
| 1 | YA | 811 | U |
| 1 | YA | 812 | C |
| 1 | YA | 827 | U |
| 1 | YA | 828 | U |
| 1 | YA | 857 | C |
| 1 | YA | 859 | G |
| 1 | YA | 877 | U |
| 1 | YA | 880 | G |
| 1 | YA | 886 | C |
| 1 | YA | 887 | A |
| 1 | YA | 888 | C |
| 1 | YA | 889 | C |
| 1 | YA | 890 | A |
| 1 | YA | 893 | C |
| 1 | YA | 896 | A |
| 1 | YA | 900 | A |
| 1 | YA | 901 | A |
| 1 | YA | 907 | U |
| 1 | YA | 910 | A |
| 1 | YA | 915 | C |
| 1 | YA | 917 | A |
| 1 | YA | 931 | G |
| 1 | YA | 932 | G |
| 1 | YA | 941 | A |
| 1 | YA | 945 | A |
| 1 | YA | 946 | G |
| 1 | YA | 953 | A |
| 1 | YA | 959 | A |
| 1 | YA | 961 | C |
| 1 | YA | 974 | G |
| 1 | YA | 975(A) | C |
| 1 | YA | 980 | A |
| 1 | YA | 983 | A |
| 1 | YA | 996 | A |
| 1 | YA | 1012 | U |
| 1 | YA | 1013 | C |
| 1 | YA | 1017 | G |
| 1 | YA | 1025 | G |
| 1 | YA | 1033 | U |
| 1 | YA | 1038 | C |
| 1 | YA | 1046 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | YA | 1047 | G |
| 1 | YA | 1048 | A |
| 1 | YA | 1052 | C |
| 1 | YA | 1053 | C |
| 1 | YA | 1054 | A |
| 1 | YA | 1058 | G |
| 1 | YA | 1060 | U |
| 1 | YA | 1063 | G |
| 1 | YA | 1064 | C |
| 1 | YA | 1065 | U |
| 1 | YA | 1066 | U |
| 1 | YA | 1067 | A |
| 1 | YA | 1068 | G |
| 1 | YA | 1069 | A |
| 1 | YA | 1070 | A |
| 1 | YA | 1071 | G |
| 1 | YA | 1073 | A |
| 1 | YA | 1074 | G |
| 1 | YA | 1076 | C |
| 1 | YA | 1077 | A |
| 1 | YA | 1078 | U |
| 1 | YA | 1079 | C |
| 1 | YA | 1082 | U |
| 1 | YA | 1083 | U |
| 1 | YA | 1084 | A |
| 1 | YA | 1085 | A |
| 1 | YA | 1086 | A |
| 1 | YA | 1088 | A |
| 1 | YA | 1090 | U |
| 1 | YA | 1091 | G |
| 1 | YA | 1092 | C |
| 1 | YA | 1094 | U |
| 1 | YA | 1096 | A |
| 1 | YA | 1097 | U |
| 1 | YA | 1098 | A |
| 1 | YA | 1109 | C |
| 1 | YA | 1110 | G |
| 1 | YA | 1111 | A |
| 1 | YA | 1112 | G |
| 1 | YA | 1126 | A |
| 1 | YA | 1130 | U |
| 1 | YA | 1135 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | YA | 1136 | G |
| 1 | YA | 1142(B) | A |
| 1 | YA | 1171 | G |
| 1 | YA | 1206 | G |
| 1 | YA | 1212 | G |
| 1 | YA | 1220 | A |
| 1 | YA | 1236 | G |
| 1 | YA | 1253 | A |
| 1 | YA | 1256 | G |
| 1 | YA | 1271 | G |
| 1 | YA | 1272 | A |
| 1 | YA | 1273 | U |
| 1 | YA | 1300 | U |
| 1 | YA | 1301 | A |
| 1 | YA | 1314 | C |
| 1 | YA | 1352 | U |
| 1 | YA | 1359 | A |
| 1 | YA | 1360 | A |
| 1 | YA | 1365 | A |
| 1 | YA | 1368 | G |
| 1 | YA | 1380 | G |
| 1 | YA | 1384 | A |
| 1 | YA | 1385 | G |
| 1 | YA | 1416 | G |
| 1 | YA | 1417 | C |
| 1 | YA | 1420 | U |
| 1 | YA | 1421 | G |
| 1 | YA | 1428 | C |
| 1 | YA | 1445(A) | A |
| 1 | YA | 1450(A) | G |
| 1 | YA | 1455 | G |
| 1 | YA | 1459 | G |
| 1 | YA | 1467 | C |
| 1 | YA | 1471 | A |
| 1 | YA | 1482 | G |
| 1 | YA | 1493 | C |
| 1 | YA | 1494 | A |
| 1 | YA | 1497 | U |
| 1 | YA | 1508 | A |
| 1 | YA | 1509(A) | C |
| 1 | YA | 1509(B) | A |
| 1 | YA | 1531 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | YA | 1542 | A |
| 1 | YA | 1543 | C |
| 1 | YA | 1547 | C |
| 1 | YA | 1558 | A |
| 1 | YA | 1559 | G |
| 1 | YA | 1566 | A |
| 1 | YA | 1569 | A |
| 1 | YA | 1578 | U |
| 1 | YA | 1580 | A |
| 1 | YA | 1584 | C |
| 1 | YA | 1586 | A |
| 1 | YA | 1608 | A |
| 1 | YA | 1609 | A |
| 1 | YA | 1610 | A |
| 1 | YA | 1640 | C |
| 1 | YA | 1648 | C |
| 1 | YA | 1674 | G |
| 1 | YA | 1696 | G |
| 1 | YA | 1700 | A |
| 1 | YA | 1701 | A |
| 1 | YA | 1721 | G |
| 1 | YA | 1722 | A |
| 1 | YA | 1750 | G |
| 1 | YA | 1756 | G |
| 1 | YA | 1762 | A |
| 1 | YA | 1763 | G |
| 1 | YA | 1764 | G |
| 1 | YA | 1773 | A |
| 1 | YA | 1780 | A |
| 1 | YA | 1786 | A |
| 1 | YA | 1791 | A |
| 1 | YA | 1800 | C |
| 1 | YA | 1801 | G |
| 1 | YA | 1812 | A |
| 1 | YA | 1816 | G |
| 1 | YA | 1835 | G |
| 1 | YA | 1847 | A |
| 1 | YA | 1848 | A |
| 1 | YA | 1877 | A |
| 1 | YA | 1878 | G |
| 1 | YA | 1900 | A |
| 1 | YA | 1906 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | YA | 1914 | C |
| 1 | YA | 1915 | 5MU |
| 1 | YA | 1927 | A |
| 1 | YA | 1929 | G |
| 1 | YA | 1930 | G |
| 1 | YA | 1936 | A |
| 1 | YA | 1938 | A |
| 1 | YA | 1955 | U |
| 1 | YA | 1963 | U |
| 1 | YA | 1967 | C |
| 1 | YA | 1970 | A |
| 1 | YA | 1971 | A |
| 1 | YA | 1972 | A |
| 1 | YA | 1975 | G |
| 1 | YA | 1993 | U |
| 1 | YA | 1997 | G |
| 1 | YA | 2023 | G |
| 1 | YA | 2031 | A |
| 1 | YA | 2032 | G |
| 1 | YA | 2033 | A |
| 1 | YA | 2043 | C |
| 1 | YA | 2055 | C |
| 1 | YA | 2056 | G |
| 1 | YA | 2060 | A |
| 1 | YA | 2061 | G |
| 1 | YA | 2062 | A |
| 1 | YA | 2069 | G |
| 1 | YA | 2096 | U |
| 1 | YA | 2099 | U |
| 1 | YA | 2103 | C |
| 1 | YA | 2104 | G |
| 1 | YA | 2105 | C |
| 1 | YA | 2107 | C |
| 1 | YA | 2108 | C |
| 1 | YA | 2109 | U |
| 1 | YA | 2112 | G |
| 1 | YA | 2115 | G |
| 1 | YA | 2116 | G |
| 1 | YA | 2117 | A |
| 1 | YA | 2118 | U |
| 1 | YA | 2119 | A |
| 1 | YA | 2121 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | YA | 2123 | G |
| 1 | YA | 2127 | G |
| 1 | YA | 2128 | C |
| 1 | YA | 2129 | C |
| 1 | YA | 2131 | G |
| 1 | YA | 2132 | U |
| 1 | YA | 2133 | G |
| 1 | YA | 2134 | A |
| 1 | YA | 2136 | C |
| 1 | YA | 2138 | C |
| 1 | YA | 2145 | C |
| 1 | YA | 2146 | C |
| 1 | YA | 2147 | G |
| 1 | YA | 2148 | G |
| 1 | YA | 2151 | G |
| 1 | YA | 2158 | A |
| 1 | YA | 2159 | G |
| 1 | YA | 2161 | C |
| 1 | YA | 2163 | C |
| 1 | YA | 2165 | G |
| 1 | YA | 2172 | U |
| 1 | YA | 2173 | A |
| 1 | YA | 2180 | U |
| 1 | YA | 2186 | G |
| 1 | YA | 2189 | U |
| 1 | YA | 2192 | G |
| 1 | YA | 2198 | A |
| 1 | YA | 2206 | G |
| 1 | YA | 2207 | G |
| 1 | YA | 2208 | A |
| 1 | YA | 2218 | U |
| 1 | YA | 2225 | A |
| 1 | YA | 2238 | G |
| 1 | YA | 2239 | G |
| 1 | YA | 2269 | A |
| 1 | YA | 2275 | C |
| 1 | YA | 2278 | A |
| 1 | YA | 2283 | C |
| 1 | YA | 2287 | A |
| 1 | YA | 2289 | G |
| 1 | YA | 2291 | U |
| 1 | YA | 2305 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | YA | 2308 | G |
| 1 | YA | 2312 | U |
| 1 | YA | 2320 | A |
| 1 | YA | 2321 | G |
| 1 | YA | 2322 | A |
| 1 | YA | 2325 | G |
| 1 | YA | 2334 | G |
| 1 | YA | 2335 | A |
| 1 | YA | 2343 | C |
| 1 | YA | 2347 | C |
| 1 | YA | 2350 | C |
| 1 | YA | 2372 | G |
| 1 | YA | 2379 | G |
| 1 | YA | 2383 | G |
| 1 | YA | 2385 | C |
| 1 | YA | 2406 | U |
| 1 | YA | 2410 | G |
| 1 | YA | 2422 | A |
| 1 | YA | 2425 | A |
| 1 | YA | 2429 | G |
| 1 | YA | 2430 | A |
| 1 | YA | 2434 | A |
| 1 | YA | 2435 | A |
| 1 | YA | 2439 | A |
| 1 | YA | 2441 | C |
| 1 | YA | 2448 | A |
| 1 | YA | 2465 | C |
| 1 | YA | 2466 | C |
| 1 | YA | 2474 | C |
| 1 | YA | 2476 | A |
| 1 | YA | 2478 | A |
| 1 | YA | 2502 | G |
| 1 | YA | 2504 | U |
| 1 | YA | 2505 | G |
| 1 | YA | 2506 | U |
| 1 | YA | 2518 | A |
| 1 | YA | 2527 | C |
| 1 | YA | 2529 | G |
| 1 | YA | 2554 | U |
| 1 | YA | 2555 | U |
| 1 | YA | 2566 | A |
| 1 | YA | 2567 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | YA | 2573 | C |
| 1 | YA | 2602 | A |
| 1 | YA | 2609 | U |
| 1 | YA | 2611 | U |
| 1 | YA | 2612 | C |
| 1 | YA | 2615 | U |
| 1 | YA | 2629 | A |
| 1 | YA | 2630 | G |
| 1 | YA | 2654 | A |
| 1 | YA | 2663 | G |
| 1 | YA | 2689 | U |
| 1 | YA | 2690 | C |
| 1 | YA | 2702 | U |
| 1 | YA | 2703 | C |
| 1 | YA | 2712(B) | A |
| 1 | YA | 2713 | A |
| 1 | YA | 2714 | G |
| 1 | YA | 2726 | U |
| 1 | YA | 2732 | G |
| 1 | YA | 2733 | A |
| 1 | YA | 2744 | G |
| 1 | YA | 2751 | G |
| 1 | YA | 2757 | A |
| 1 | YA | 2758 | A |
| 1 | YA | 2759 | G |
| 1 | YA | 2764 | A |
| 1 | YA | 2765 | A |
| 1 | YA | 2766 | G |
| 1 | YA | 2769 | C |
| 1 | YA | 2778 | A |
| 1 | YA | 2780 | G |
| 1 | YA | 2811 | G |
| 1 | YA | 2818 | G |
| 1 | YA | 2820 | A |
| 1 | YA | 2821 | A |
| 1 | YA | 2833 | G |
| 1 | YA | 2849 | U |
| 1 | YA | 2872 | G |
| 1 | YA | 2873 | A |
| 1 | YA | 2880 | C |
| 1 | YA | 2886 | G |
| 1 | YA | 2892 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | YA | 2894 | G |
| 1 | YA | 2897 | U |
| 2 | YB | 2 | C |
| 2 | YB | 8 | U |
| 2 | YB | 9 | G |
| 2 | YB | 13 | A |
| 2 | YB | 30 | C |
| 2 | YB | 56 | G |
| 2 | YB | 73 | A |
| 2 | YB | 84 | C |
| 2 | YB | 106 | G |
| 2 | YB | 110 | G |
| 32 | XA | 5 | U |
| 32 | XA | 7 | G |
| 32 | XA | 9 | G |
| 32 | XA | 32 | A |
| 32 | XA | 39 | G |
| 32 | XA | 47 | C |
| 32 | XA | 48 | C |
| 32 | XA | 50 | A |
| 32 | XA | 51 | A |
| 32 | XA | 61 | G |
| 32 | XA | 66 | G |
| 32 | XA | 88 | A |
| 32 | XA | 89 | C |
| 32 | XA | 101 | A |
| 32 | XA | 116 | A |
| 32 | XA | 121 | C |
| 32 | XA | 131 | C |
| 32 | XA | 156 | G |
| 32 | XA | 163 | C |
| 32 | XA | 174 | C |
| 32 | XA | 182 | U |
| 32 | XA | 189(F) | U |
| 32 | XA | 195 | A |
| 32 | XA | 197 | A |
| 32 | XA | 202 | U |
| 32 | XA | 203 | U |
| 32 | XA | 204 | U |
| 32 | XA | 216 | G |
| 32 | XA | 247 | G |
| 32 | XA | 251 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | XA | 266 | G |
| 32 | XA | 267 | C |
| 32 | XA | 289 | G |
| 32 | XA | 318 | G |
| 32 | XA | 321 | A |
| 32 | XA | 328 | C |
| 32 | XA | 332 | G |
| 32 | XA | 348 | G |
| 32 | XA | 350 | G |
| 32 | XA | 352 | C |
| 32 | XA | 353 | A |
| 32 | XA | 354 | G |
| 32 | XA | 367 | U |
| 32 | XA | 372 | C |
| 32 | XA | 373 | A |
| 32 | XA | 384 | G |
| 32 | XA | 397 | A |
| 32 | XA | 398 | C |
| 32 | XA | 406 | G |
| 32 | XA | 412 | A |
| 32 | XA | 413 | G |
| 32 | XA | 424 | G |
| 32 | XA | 429 | U |
| 32 | XA | 439 | A |
| 32 | XA | 442 | C |
| 32 | XA | 452 | A |
| 32 | XA | 458 | C |
| 32 | XA | 461 | A |
| 32 | XA | 470 | C |
| 32 | XA | 485 | G |
| 32 | XA | 496 | A |
| 32 | XA | 498 | U |
| 32 | XA | 505 | G |
| 32 | XA | 509 | A |
| 32 | XA | 510 | A |
| 32 | XA | 511 | C |
| 32 | XA | 518 | C |
| 32 | XA | 521 | G |
| 32 | XA | 527 | 7MG |
| 32 | XA | 532 | A |
| 32 | XA | 533 | A |
| 32 | XA | 547 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | XA | 559 | A |
| 32 | XA | 561 | U |
| 32 | XA | 564 | C |
| 32 | XA | 572 | A |
| 32 | XA | 573 | A |
| 32 | XA | 575 | G |
| 32 | XA | 576 | G |
| 32 | XA | 577 | G |
| 32 | XA | 592 | G |
| 32 | XA | 596 | C |
| 32 | XA | 630 | G |
| 32 | XA | 631 | G |
| 32 | XA | 632 | A |
| 32 | XA | 653 | A |
| 32 | XA | 661 | G |
| 32 | XA | 665 | A |
| 32 | XA | 687 | A |
| 32 | XA | 688 | G |
| 32 | XA | 695 | A |
| 32 | XA | 721 | G |
| 32 | XA | 723 | U |
| 32 | XA | 731 | G |
| 32 | XA | 749 | C |
| 32 | XA | 753 | A |
| 32 | XA | 755 | G |
| 32 | XA | 774 | G |
| 32 | XA | 777 | A |
| 32 | XA | 787 | A |
| 32 | XA | 792 | A |
| 32 | XA | 793 | U |
| 32 | XA | 794 | A |
| 32 | XA | 817 | C |
| 32 | XA | 818 | G |
| 32 | XA | 821 | G |
| 32 | XA | 828 | A |
| 32 | XA | 829 | G |
| 32 | XA | 840 | C |
| 32 | XA | 841 | U |
| 32 | XA | 848 | C |
| 32 | XA | 851 | G |
| 32 | XA | 902 | G |
| 32 | XA | 914 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | XA | 926 | G |
| 32 | XA | 927 | G |
| 32 | XA | 931 | C |
| 32 | XA | 934 | C |
| 32 | XA | 942 | G |
| 32 | XA | 960 | U |
| 32 | XA | 961 | U |
| 32 | XA | 968 | A |
| 32 | XA | 969 | A |
| 32 | XA | 971 | G |
| 32 | XA | 972 | C |
| 32 | XA | 974 | A |
| 32 | XA | 975 | A |
| 32 | XA | 976 | G |
| 32 | XA | 977 | A |
| 32 | XA | 992 | U |
| 32 | XA | 993 | G |
| 32 | XA | 994 | A |
| 32 | XA | 999 | C |
| 32 | XA | 1003 | G |
| 32 | XA | 1004 | A |
| 32 | XA | 1005 | A |
| 32 | XA | 1006 | C |
| 32 | XA | 1009 | G |
| 32 | XA | 1020 | U |
| 32 | XA | 1022 | G |
| 32 | XA | 1023 | G |
| 32 | XA | 1025 | U |
| 32 | XA | 1026 | G |
| 32 | XA | 1027 | C |
| 32 | XA | 1028 | C |
| 32 | XA | 1029 | C |
| 32 | XA | 1030(B) | G |
| 32 | XA | 1030(C) | C |
| 32 | XA | 1033 | G |
| 32 | XA | 1036 | G |
| 32 | XA | 1041 | A |
| 32 | XA | 1044 | A |
| 32 | XA | 1054 | C |
| 32 | XA | 1055 | A |
| 32 | XA | 1065 | U |
| 32 | XA | 1066 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | XA | 1068 | G |
| 32 | XA | 1081 | G |
| 32 | XA | 1094 | G |
| 32 | XA | 1095 | U |
| 32 | XA | 1101 | A |
| 32 | XA | 1117 | G |
| 32 | XA | 1125 | U |
| 32 | XA | 1129 | C |
| 32 | XA | 1130 | A |
| 32 | XA | 1136 | U |
| 32 | XA | 1137 | C |
| 32 | XA | 1138 | G |
| 32 | XA | 1139 | G |
| 32 | XA | 1140 | C |
| 32 | XA | 1147 | C |
| 32 | XA | 1152 | A |
| 32 | XA | 1159 | U |
| 32 | XA | 1183 | A |
| 32 | XA | 1184 | G |
| 32 | XA | 1196 | U |
| 32 | XA | 1197 | G |
| 32 | XA | 1211 | U |
| 32 | XA | 1212 | U |
| 32 | XA | 1213 | A |
| 32 | XA | 1224 | G |
| 32 | XA | 1227 | A |
| 32 | XA | 1236 | A |
| 32 | XA | 1238 | A |
| 32 | XA | 1250 | A |
| 32 | XA | 1256 | A |
| 32 | XA | 1257 | U |
| 32 | XA | 1258 | G |
| 32 | XA | 1278 | U |
| 32 | XA | 1279 | A |
| 32 | XA | 1280 | A |
| 32 | XA | 1281 | U |
| 32 | XA | 1286 | A |
| 32 | XA | 1287 | A |
| 32 | XA | 1300 | G |
| 32 | XA | 1305 | G |
| 32 | XA | 1320 | C |
| 32 | XA | 1340 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | XA | 1347 | G |
| 32 | XA | 1353 | G |
| 32 | XA | 1363(A) | C |
| 32 | XA | 1364 | U |
| 32 | XA | 1370 | G |
| 32 | XA | 1394 | A |
| 32 | XA | 1397 | C |
| 32 | XA | 1399 | C |
| 32 | XA | 1401 | G |
| 32 | XA | 1419 | G |
| 32 | XA | 1442(A) | G |
| 32 | XA | 1442(B) | G |
| 32 | XA | 1446 | U |
| 32 | XA | 1447 | A |
| 32 | XA | 1452 | C |
| 32 | XA | 1487 | G |
| 32 | XA | 1492 | A |
| 32 | XA | 1493 | A |
| 32 | XA | 1497 | G |
| 32 | XA | 1499 | A |
| 32 | XA | 1503 | A |
| 32 | XA | 1504 | G |
| 32 | XA | 1506 | U |
| 32 | XA | 1517 | G |
| 32 | XA | 1520 | G |
| 32 | XA | 1525 | G |
| 32 | XA | 1529 | G |
| 32 | XA | 1530 | G |
| 32 | XA | 1531 | A |
| 53 | XV | 2 | G |
| 53 | XV | 4 | G |
| 53 | XV | 5 | G |
| 53 | XV | 9 | G |
| 53 | XV | 17(A) | U |
| 53 | XV | 18 | G |
| 53 | XV | 19 | G |
| 53 | XV | 21 | A |
| 53 | XV | 31 | G |
| 53 | XV | 47 | U |
| 53 | XV | 48 | C |
| 53 | XV | 52 | G |
| 53 | XV | 53 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | XV | 54 | U |
| 53 | XV | 76 | A |
| 54 | XX | 15 | A |
| 54 | XX | 21 | A |
| 54 | XX | 22 | C |

All (88) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | RA | 9 | U |
| 1 | RA | 196 | A |
| 1 | RA | 272(M) | G |
| 1 | RA | 277 | C |
| 1 | RA | 752 | A |
| 1 | RA | 856 | C |
| 1 | RA | 900 | A |
| 1 | RA | 1047 | G |
| 1 | RA | 1053 | C |
| 1 | RA | 1057 | A |
| 1 | RA | 1065 | U |
| 1 | RA | 1067 | A |
| 1 | RA | 1073 | A |
| 1 | RA | 1076 | C |
| 1 | RA | 1210 | A |
| 1 | RA | 1379 | A |
| 1 | RA | 1420 | U |
| 1 | RA | 1530 | C |
| 1 | RA | 1913 | A |
| 1 | RA | 1992 | G |
| 1 | RA | 2126 | A |
| 1 | RA | 2171 | A |
| 1 | RA | 2172 | U |
| 1 | RA | 2321 | G |
| 1 | RA | 2573 | C |
| 1 | RA | 2689 | U |
| 1 | RA | 2756 | U |
| 32 | QA | 115 | G |
| 32 | QA | 266 | G |
| 32 | QA | 509 | A |
| 32 | QA | 560 | U |
| 32 | QA | 687 | A |
| 32 | QA | 839 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | QA | 913 | A |
| 32 | QA | 991 | U |
| 32 | QA | 1065 | U |
| 32 | QA | 1067 | A |
| 32 | QA | 1201 | A |
| 32 | QA | 1207 | 2MG |
| 32 | QA | 1256 | A |
| 32 | QA | 1281 | U |
| 32 | QA | 1285 | A |
| 32 | QA | 1442(A) | G |
| 1 | YA | 9 | U |
| 1 | YA | 196 | A |
| 1 | YA | 272(M) | G |
| 1 | YA | 277 | C |
| 1 | YA | 752 | A |
| 1 | YA | 827 | U |
| 1 | YA | 856 | C |
| 1 | YA | 900 | A |
| 1 | YA | 1047 | G |
| 1 | YA | 1053 | C |
| 1 | YA | 1057 | A |
| 1 | YA | 1065 | U |
| 1 | YA | 1067 | A |
| 1 | YA | 1073 | A |
| 1 | YA | 1076 | C |
| 1 | YA | 1379 | A |
| 1 | YA | 1420 | U |
| 1 | YA | 1530 | C |
| 1 | YA | 1992 | G |
| 1 | YA | 2126 | A |
| 1 | YA | 2171 | A |
| 1 | YA | 2172 | U |
| 1 | YA | 2321 | G |
| 1 | YA | 2689 | U |
| 1 | YA | 2756 | U |
| 32 | XA | 60 | A |
| 32 | XA | 65 | U |
| 32 | XA | 115 | G |
| 32 | XA | 266 | G |
| 32 | XA | 509 | A |
| 32 | XA | 560 | U |
| 32 | XA | 687 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | XA | 748 | C |
| 32 | XA | 840 | C |
| 32 | XA | 913 | A |
| 32 | XA | 991 | U |
| 32 | XA | 992 | U |
| 32 | XA | 1065 | U |
| 32 | XA | 1067 | A |
| 32 | XA | 1128 | C |
| 32 | XA | 1212 | U |
| 32 | XA | 1256 | A |
| 32 | XA | 1279 | A |
| 32 | XA | 1442(A) | G |
| 53 | XV | 53 | G |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 32 | 2MG | QA | 1207 | 32,56 | 18,26,27 | 3.81 | 6 (33%) | 21,38,41 | 2.64 | 7 (33%) |
| 32 | 5MC | QA | 1400 | 32 | 14,22,23 | 3.22 | 5 (35%) | 17,32,35 | 0.91 | 0 |
| 32 | 4OC | QA | 1402 | 32 | 15,23,24 | 3.49 | 5 (33%) | 21,32,35 | 2.02 | 3 (14%) |
| 32 | 5MC | QA | 1404 | 32 | 14,22,23 | 3.22 | 5 (35%) | 17,32,35 | 0.98 | 2 (11%) |
| 32 | 5MC | QA | 1407 | 32 | 14,22,23 | 3.21 | 5 (35%) | 17,32,35 | 1.01 | 1 (5%) |
| 32 | UR3 | QA | 1498 | 32 | 13,22,23 | 3.52 | 3 (23%) | 18,32,35 | 0.73 | 0 |
| 32 | MA6 | QA | 1518 | 32 | 18,26,27 | 1.10 | 2 (11%) | 15,38,41 | 2.90 | 2 (13%) |
| 32 | MA6 | QA | 1519 | 32 | 18,26,27 | 1.10 | 2 (11%) | 15,38,41 | 2.65 | 2 (13%) |
| 32 | PSU | QA | 516 | 32,56 | 15,21,22 | 3.76 | 7 (46%) | 16,30,33 | 1.84 | 3 (18%) |
| 32 | 7MG | QA | 527 | 32,56 | 20,26,27 | 4.64 | 8 (40%) | 23,39,42 | 2.25 | 8 (34%) |
| 32 | M2G | QA | 966 | 32 | 18,27,28 | 3.99 | 5 (27%) | 22,40,43 | 3.38 | 7 (31%) |
| 32 | 5MC | QA | 967 | 32 | 14,22,23 | 3.28 | 5 (35%) | 17,32,35 | 0.79 | 1 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 43 | 0TD | QL | 92 | 43 | 4,9,10 | 1.08 | 0 | 4,11,13 | 2.84 | 2 (50%) |
| 55 | MEQ | QY | 235 | 55 | 7,9,10 | 0.79 | 0 | 8,10,12 | 1.02 | 1 (12%) |
| 1 | PSU | RA | 1911 | 1 | 15,21,22 | 3.79 | 7 (46%) | 16,30,33 | 1.91 | 3 (18%) |
| 1 | 5MU | RA | 1915 | 1 | 13,22,23 | 1.60 | 2 (15%) | 16,32,35 | 1.65 | 2 (12%) |
| 1 | PSU | RA | 1917 | 1 | 15,21,22 | 3.79 | 7 (46%) | 16,30,33 | 2.04 | 4 (25%) |
| 1 | 4OC | RA | 1920 | 1 | 15,22,24 | 3.50 | 6 (40%) | 20,31,35 | 1.57 | 2 (10%) |
| 1 | 5MU | RA | 1939 | 1 | 13,22,23 | 1.41 | 2 (15%) | 16,32,35 | 1.67 | 2 (12%) |
| 1 | 5MC | RA | 1942 | 1,56 | 14,22,23 | 3.28 | 5 (35%) | 17,32,35 | 0.85 | 1 (5%) |
| 1 | 5MC | RA | 1962 | 1,56 | 14,22,23 | 3.24 | 5 (35%) | 17,32,35 | 0.82 | 1 (5%) |
| 1 | OMG | RA | 2251 | 1,56,53 | 18,26,27 | 3.33 | 6 (33%) | 21,38,41 | 2.56 | 6 (28%) |
| 1 | 2MA | RA | 2503 | 1,56 | 17,25,26 | 3.99 | 5 (29%) | 18,37,40 | 4.48 | 4 (22%) |
| 1 | 2MU | RA | 2552 | 1,56 | 14,22,24 | 8.18 | 9 (64%) | 19,31,36 | 1.37 | 2 (10%) |
| 1 | PSU | RA | 2605 | 1 | 15,21,22 | 3.77 | 7 (46%) | 16,30,33 | 1.91 | 4 (25%) |
| 32 | 2MG | XA | 1207 | 32 | 18,26,27 | 3.77 | 6 (33%) | 21,38,41 | 2.46 | 6 (28%) |
| 32 | 5MC | XA | 1400 | 32 | 14,22,23 | 3.23 | 5 (35%) | 17,32,35 | 0.84 | 1 (5%) |
| 32 | 4OC | XA | 1402 | 32 | 15,23,24 | 3.34 | 5 (33%) | 21,32,35 | 2.84 | 3 (14%) |
| 32 | 5MC | XA | 1404 | 32 | 14,22,23 | 3.17 | 5 (35%) | 17,32,35 | 0.90 | 1 (5%) |
| 32 | 5MC | XA | 1407 | 32 | 14,22,23 | 3.22 | 5 (35%) | 17,32,35 | 0.91 | 1 (5%) |
| 32 | UR3 | XA | 1498 | 32,56 | 13,22,23 | 3.55 | 3 (23%) | 18,32,35 | 0.73 | 0 |
| 32 | MA6 | XA | 1518 | 32 | 18,26,27 | 1.04 | 2 (11%) | 15,38,41 | 2.84 | 2 (13%) |
| 32 | MA6 | XA | 1519 | 32 | 18,26,27 | 1.06 | 2 (11%) | 15,38,41 | 3.03 | 3 (20%) |
| 32 | PSU | XA | 516 | 32 | 15,21,22 | 3.78 | 7 (46%) | 16,30,33 | 1.95 | 3 (18%) |
| 32 | 7MG | XA | 527 | 32,56 | 20,26,27 | 4.65 | 9 (45%) | 23,39,42 | 2.23 | 8 (34%) |
| 32 | M2G | XA | 966 | 32 | 18,27,28 | 3.93 | 5 (27%) | 22,40,43 | 3.21 | 6 (27%) |
| 32 | 5MC | XA | 967 | 32 | 14,22,23 | 3.23 | 5 (35%) | 17,32,35 | 0.90 | 1 (5%) |
| 43 | 0TD | XL | 92 | 43 | 4,9,10 | 1.08 | 0 | 4,11,13 | 2.76 | 2 (50%) |
| 55 | MEQ | XY | 235 | 55 | 7,9,10 | 0.81 | 0 | 8,10,12 | 0.81 | 0 |
| 1 | PSU | YA | 1911 | 1 | 15,21,22 | 3.78 | 7 (46%) | 16,30,33 | 1.98 | 4 (25%) |
| 1 | 5MU | YA | 1915 | 1,56 | 13,22,23 | 1.56 | 2 (15%) | 16,32,35 | 1.69 | 3 (18%) |
| 1 | PSU | YA | 1917 | 1 | 15,21,22 | 3.76 | 7 (46%) | 16,30,33 | 1.97 | 4 (25%) |
| 1 | 4OC | YA | 1920 | 1 | 15,22,24 | 3.47 | 6 (40%) | 20,31,35 | 1.63 | 2 (10%) |
| 1 | 5MU | YA | 1939 | 1,56 | 13,22,23 | 1.38 | 2 (15%) | 16,32,35 | 1.81 | 3 (18%) |
| 1 | 5MC | YA | 1942 | 1 | 14,22,23 | 3.27 | 5 (35%) | 17,32,35 | 0.90 | 1 (5%) |
| 1 | 5MC | YA | 1962 | 1,56 | 14,22,23 | 3.25 | 5 (35%) | 17,32,35 | 0.83 | 1 (5%) |
| 1 | OMG | YA | 2251 | 1,56,53 | 18,26,27 | 3.30 | 6 (33%) | 21,38,41 | 2.51 | 6 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 2MA | YA | 2503 | 1,56 | 17,25,26 | 4.04 | 5 (29%) | 18,37,40 | 4.44 | 4 (22%) |
| 1 | 2MU | YA | 2552 | 1,56 | 14,22,24 | 8.21 | 9 (64%) | 19,31,36 | 1.42 | 2 (10%) |
| 1 | PSU | YA | 2605 | 1 | 15,21,22 | 3.74 | 7 (46%) | 16,30,33 | 1.84 | 4 (25%) |

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 |
|-----|------|-------|------|---------|---------|-----------|---------|
| 32 | 2MG | QA | 1207 | 32,56 | - | 0/5/27/28 | 0/3/3/3 |
| 32 | 5MC | QA | 1400 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | 4OC | QA | 1402 | 32 | - | 0/7/29/30 | 0/2/2/2 |
| 32 | 5MC | QA | 1404 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | 5MC | QA | 1407 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | UR3 | QA | 1498 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | MA6 | QA | 1518 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | MA6 | QA | 1519 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | PSU | QA | 516 | 32,56 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | QA | 527 | 32,56 | - | 0/7/37/38 | 0/3/3/3 |
| 32 | M2G | QA | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | 5MC | QA | 967 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 43 | 0TD | QL | 92 | 43 | - | 0/2/12/14 | 0/0/0/0 |
| 55 | MEQ | QY | 235 | 55 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | PSU | RA | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | RA | 1915 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | PSU | RA | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | RA | 1920 | 1 | - | 0/5/27/30 | 0/2/2/2 |
| 1 | 5MU | RA | 1939 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 5MC | RA | 1942 | 1,56 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 5MC | RA | 1962 | 1,56 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | OMG | RA | 2251 | 1,56,53 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 2MA | RA | 2503 | 1,56 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | 2MU | RA | 2552 | 1,56 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | PSU | RA | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | XA | 1207 | 32 | - | 0/5/27/28 | 0/3/3/3 |
| 32 | 5MC | XA | 1400 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | 4OC | XA | 1402 | 32 | - | 0/7/29/30 | 0/2/2/2 |
| 32 | 5MC | XA | 1404 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | 5MC | XA | 1407 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | UR3 | XA | 1498 | 32,56 | - | 0/3/25/26 | 0/2/2/2 |
| 32 | MA6 | XA | 1518 | 32 | - | 0/7/29/30 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|-----------|---------|
| 32 | MA6 | XA | 1519 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | PSU | XA | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | XA | 527 | 32,56 | - | 0/7/37/38 | 0/3/3/3 |
| 32 | M2G | XA | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | 5MC | XA | 967 | 32 | - | 0/3/25/26 | 0/2/2/2 |
| 43 | 0TD | XL | 92 | 43 | - | 0/2/12/14 | 0/0/0/0 |
| 55 | MEQ | XY | 235 | 55 | - | 0/7/9/11 | 0/0/0/0 |
| 1 | PSU | YA | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | YA | 1915 | 1,56 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | PSU | YA | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | YA | 1920 | 1 | - | 0/5/27/30 | 0/2/2/2 |
| 1 | 5MU | YA | 1939 | 1,56 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 5MC | YA | 1942 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 5MC | YA | 1962 | 1,56 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | OMG | YA | 2251 | 1,56,53 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 2MA | YA | 2503 | 1,56 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | 2MU | YA | 2552 | 1,56 | - | 0/5/27/28 | 0/2/2/2 |
| 1 | PSU | YA | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |

All (239) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | YA | 2552 | 2MU | C6-C5 | -9.51 | 1.17 | 1.38 |
| 1 | RA | 2552 | 2MU | C6-C5 | -9.50 | 1.17 | 1.38 |
| 1 | YA | 2552 | 2MU | C3'-C2' | -8.51 | 1.33 | 1.53 |
| 1 | RA | 2552 | 2MU | C3'-C2' | -8.26 | 1.34 | 1.53 |
| 1 | RA | 2552 | 2MU | C4-N3 | -6.87 | 1.20 | 1.33 |
| 1 | YA | 2552 | 2MU | C4-N3 | -6.87 | 1.20 | 1.33 |
| 1 | YA | 2552 | 2MU | O4'-C4' | -5.41 | 1.32 | 1.45 |
| 1 | RA | 2552 | 2MU | O4'-C4' | -5.34 | 1.32 | 1.45 |
| 1 | RA | 1915 | 5MU | C4-N3 | -4.50 | 1.24 | 1.33 |
| 1 | YA | 1915 | 5MU | C4-N3 | -4.33 | 1.25 | 1.33 |
| 1 | YA | 1911 | PSU | C5-C1' | -4.30 | 1.48 | 1.52 |
| 32 | XA | 516 | PSU | C5-C1' | -4.20 | 1.48 | 1.52 |
| 1 | RA | 1917 | PSU | C5-C1' | -3.81 | 1.48 | 1.52 |
| 1 | RA | 1939 | 5MU | C4-N3 | -3.78 | 1.26 | 1.33 |
| 1 | YA | 1917 | PSU | C5-C1' | -3.77 | 1.49 | 1.52 |
| 1 | YA | 1939 | 5MU | C4-N3 | -3.63 | 1.26 | 1.33 |
| 1 | RA | 1911 | PSU | C5-C1' | -3.60 | 1.49 | 1.52 |
| 1 | RA | 2605 | PSU | C5-C1' | -3.53 | 1.49 | 1.52 |
| 1 | YA | 2605 | PSU | C5-C1' | -3.52 | 1.49 | 1.52 |
| 1 | YA | 2251 | OMG | O6-C6 | -3.28 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | RA | 2251 | OMG | O6-C6 | -3.26 | 1.16 | 1.24 |
| 32 | QA | 516 | PSU | C5-C1' | -3.19 | 1.49 | 1.52 |
| 32 | QA | 1519 | MA6 | C5-C4 | -2.45 | 1.35 | 1.40 |
| 32 | XA | 1518 | MA6 | C5-C4 | -2.42 | 1.35 | 1.40 |
| 32 | QA | 1518 | MA6 | C5-C4 | -2.37 | 1.35 | 1.40 |
| 32 | XA | 1519 | MA6 | C5-C4 | -2.29 | 1.35 | 1.40 |
| 32 | QA | 516 | PSU | O4-C4 | -2.24 | 1.18 | 1.24 |
| 1 | RA | 2605 | PSU | O4-C4 | -2.24 | 1.18 | 1.24 |
| 1 | YA | 2605 | PSU | O4-C4 | -2.19 | 1.19 | 1.24 |
| 1 | RA | 1911 | PSU | O4-C4 | -2.17 | 1.19 | 1.24 |
| 32 | XA | 516 | PSU | O4-C4 | -2.15 | 1.19 | 1.24 |
| 1 | RA | 1917 | PSU | O4-C4 | -2.13 | 1.19 | 1.24 |
| 1 | YA | 1917 | PSU | O4-C4 | -2.10 | 1.19 | 1.24 |
| 1 | YA | 1911 | PSU | O4-C4 | -2.08 | 1.19 | 1.24 |
| 32 | XA | 527 | 7MG | C8-N7 | 2.06 | 1.53 | 1.43 |
| 32 | XA | 1518 | MA6 | C2-N3 | 2.21 | 1.36 | 1.32 |
| 32 | XA | 1519 | MA6 | C2-N3 | 2.22 | 1.36 | 1.32 |
| 1 | YA | 1939 | 5MU | C6-C5 | 2.25 | 1.46 | 1.40 |
| 1 | YA | 2552 | 2MU | O2'-C2' | 2.34 | 1.49 | 1.42 |
| 1 | RA | 1939 | 5MU | C6-C5 | 2.35 | 1.46 | 1.40 |
| 32 | QA | 1518 | MA6 | C2-N3 | 2.37 | 1.36 | 1.32 |
| 1 | RA | 2552 | 2MU | O2'-C2' | 2.37 | 1.49 | 1.42 |
| 32 | QA | 1519 | MA6 | C2-N3 | 2.42 | 1.36 | 1.32 |
| 1 | YA | 1915 | 5MU | C6-C5 | 2.44 | 1.46 | 1.40 |
| 1 | RA | 1915 | 5MU | C6-C5 | 2.48 | 1.46 | 1.40 |
| 32 | XA | 527 | 7MG | C5-C4 | 2.50 | 1.45 | 1.39 |
| 32 | QA | 527 | 7MG | C5-C4 | 2.67 | 1.46 | 1.39 |
| 32 | QA | 1207 | 2MG | C2-N1 | 3.02 | 1.45 | 1.34 |
| 32 | XA | 1207 | 2MG | C2-N1 | 3.03 | 1.45 | 1.34 |
| 32 | XA | 1207 | 2MG | C2-N3 | 3.30 | 1.46 | 1.34 |
| 32 | QA | 1207 | 2MG | C2-N3 | 3.32 | 1.46 | 1.34 |
| 1 | RA | 2552 | 2MU | C2-N3 | 3.34 | 1.45 | 1.38 |
| 1 | YA | 2552 | 2MU | C2-N3 | 3.41 | 1.45 | 1.38 |
| 1 | YA | 1962 | 5MC | C6-C5 | 3.47 | 1.49 | 1.40 |
| 1 | RA | 1942 | 5MC | C6-C5 | 3.47 | 1.49 | 1.40 |
| 32 | XA | 1400 | 5MC | C6-C5 | 3.48 | 1.49 | 1.40 |
| 1 | YA | 1942 | 5MC | C6-C5 | 3.50 | 1.49 | 1.40 |
| 1 | RA | 1962 | 5MC | C6-C5 | 3.51 | 1.49 | 1.40 |
| 32 | XA | 1407 | 5MC | C6-C5 | 3.56 | 1.49 | 1.40 |
| 32 | QA | 1407 | 5MC | C6-C5 | 3.62 | 1.49 | 1.40 |
| 32 | QA | 967 | 5MC | C6-C5 | 3.62 | 1.49 | 1.40 |
| 1 | YA | 1920 | 4OC | C5-C4 | 3.70 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 1 | RA | 1920 | 4OC | C5-C4 | 3.72 | 1.49 | 1.41 |
| 32 | XA | 967 | 5MC | C6-C5 | 3.72 | 1.49 | 1.40 |
| 32 | QA | 1400 | 5MC | C6-C5 | 3.73 | 1.49 | 1.40 |
| 32 | XA | 1404 | 5MC | C6-C5 | 3.74 | 1.49 | 1.40 |
| 1 | YA | 1920 | 4OC | C4-N4 | 3.80 | 1.46 | 1.35 |
| 32 | QA | 1404 | 5MC | C6-C5 | 3.80 | 1.50 | 1.40 |
| 1 | RA | 1920 | 4OC | C4-N4 | 3.81 | 1.46 | 1.35 |
| 1 | YA | 2552 | 2MU | C3'-C4' | 3.88 | 1.63 | 1.53 |
| 1 | RA | 2552 | 2MU | C3'-C4' | 3.94 | 1.63 | 1.53 |
| 32 | XA | 1407 | 5MC | C4-N4 | 4.13 | 1.45 | 1.34 |
| 1 | RA | 1942 | 5MC | C4-N4 | 4.13 | 1.45 | 1.34 |
| 1 | RA | 1962 | 5MC | C4-N4 | 4.14 | 1.45 | 1.34 |
| 1 | YA | 1962 | 5MC | C4-N4 | 4.14 | 1.45 | 1.34 |
| 1 | YA | 1942 | 5MC | C4-N4 | 4.14 | 1.45 | 1.34 |
| 32 | XA | 1400 | 5MC | C4-N4 | 4.17 | 1.45 | 1.34 |
| 32 | QA | 1400 | 5MC | C4-N4 | 4.17 | 1.45 | 1.34 |
| 32 | XA | 1404 | 5MC | C4-N4 | 4.18 | 1.45 | 1.34 |
| 32 | QA | 1407 | 5MC | C4-N4 | 4.18 | 1.45 | 1.34 |
| 32 | QA | 967 | 5MC | C4-N4 | 4.19 | 1.45 | 1.34 |
| 32 | XA | 967 | 5MC | C4-N4 | 4.20 | 1.45 | 1.34 |
| 32 | QA | 1404 | 5MC | C4-N4 | 4.23 | 1.45 | 1.34 |
| 32 | XA | 1402 | 4OC | C5-C4 | 4.54 | 1.49 | 1.39 |
| 32 | QA | 1402 | 4OC | C5-C4 | 4.55 | 1.49 | 1.39 |
| 32 | XA | 1402 | 4OC | C2-N3 | 4.72 | 1.48 | 1.38 |
| 32 | XA | 516 | PSU | C6-N1 | 4.92 | 1.44 | 1.34 |
| 32 | XA | 1402 | 4OC | C6-C5 | 4.92 | 1.48 | 1.38 |
| 1 | YA | 1911 | PSU | C6-N1 | 4.93 | 1.44 | 1.34 |
| 1 | YA | 2605 | PSU | C6-N1 | 4.95 | 1.44 | 1.34 |
| 1 | YA | 1917 | PSU | C6-N1 | 4.97 | 1.44 | 1.34 |
| 1 | RA | 2605 | PSU | C6-N1 | 5.02 | 1.45 | 1.34 |
| 1 | RA | 1911 | PSU | C6-N1 | 5.05 | 1.45 | 1.34 |
| 1 | YA | 2251 | OMG | C2-N2 | 5.06 | 1.44 | 1.34 |
| 32 | XA | 1498 | UR3 | C6-C5 | 5.09 | 1.49 | 1.38 |
| 1 | RA | 2251 | OMG | C2-N2 | 5.11 | 1.44 | 1.34 |
| 32 | QA | 1402 | 4OC | C6-C5 | 5.12 | 1.49 | 1.38 |
| 1 | RA | 1917 | PSU | C6-N1 | 5.12 | 1.45 | 1.34 |
| 32 | XA | 1404 | 5MC | C2-N3 | 5.13 | 1.48 | 1.38 |
| 32 | QA | 1498 | UR3 | C6-C5 | 5.15 | 1.49 | 1.38 |
| 32 | QA | 516 | PSU | C6-N1 | 5.17 | 1.45 | 1.34 |
| 1 | YA | 1920 | 4OC | C6-C5 | 5.19 | 1.49 | 1.38 |
| 1 | RA | 2503 | 2MA | C6-N1 | 5.20 | 1.45 | 1.34 |
| 1 | RA | 1920 | 4OC | C6-C5 | 5.22 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 32 | QA | 1400 | 5MC | C2-N3 | 5.23 | 1.49 | 1.38 |
| 32 | QA | 527 | 7MG | C2-N2 | 5.23 | 1.45 | 1.34 |
| 32 | XA | 1407 | 5MC | C2-N3 | 5.24 | 1.49 | 1.38 |
| 32 | QA | 1404 | 5MC | C2-N3 | 5.24 | 1.49 | 1.38 |
| 1 | YA | 1920 | 4OC | C2-N3 | 5.27 | 1.49 | 1.38 |
| 32 | QA | 1407 | 5MC | C2-N3 | 5.27 | 1.49 | 1.38 |
| 32 | QA | 1402 | 4OC | C2-N3 | 5.27 | 1.49 | 1.38 |
| 32 | XA | 967 | 5MC | C2-N3 | 5.31 | 1.49 | 1.38 |
| 1 | YA | 2503 | 2MA | C6-N1 | 5.32 | 1.45 | 1.34 |
| 1 | RA | 1962 | 5MC | C2-N3 | 5.35 | 1.49 | 1.38 |
| 1 | RA | 1920 | 4OC | C2-N3 | 5.35 | 1.49 | 1.38 |
| 32 | XA | 527 | 7MG | C2-N2 | 5.36 | 1.45 | 1.34 |
| 1 | RA | 1942 | 5MC | C2-N3 | 5.39 | 1.49 | 1.38 |
| 32 | XA | 1400 | 5MC | C2-N3 | 5.39 | 1.49 | 1.38 |
| 32 | QA | 967 | 5MC | C2-N3 | 5.39 | 1.49 | 1.38 |
| 1 | YA | 1962 | 5MC | C2-N3 | 5.43 | 1.49 | 1.38 |
| 32 | QA | 516 | PSU | C2-N3 | 5.43 | 1.49 | 1.38 |
| 1 | RA | 2605 | PSU | C2-N3 | 5.44 | 1.49 | 1.38 |
| 32 | QA | 527 | 7MG | C8-N9 | 5.44 | 1.53 | 1.45 |
| 1 | YA | 1962 | 5MC | C5-C4 | 5.45 | 1.49 | 1.41 |
| 1 | YA | 1942 | 5MC | C2-N3 | 5.49 | 1.49 | 1.38 |
| 32 | XA | 527 | 7MG | C8-N9 | 5.50 | 1.53 | 1.45 |
| 32 | XA | 516 | PSU | C2-N3 | 5.52 | 1.49 | 1.38 |
| 1 | YA | 2605 | PSU | C2-N3 | 5.53 | 1.49 | 1.38 |
| 1 | YA | 1917 | PSU | C2-N3 | 5.54 | 1.49 | 1.38 |
| 1 | YA | 1911 | PSU | C2-N3 | 5.55 | 1.49 | 1.38 |
| 1 | RA | 1911 | PSU | C2-N3 | 5.55 | 1.49 | 1.38 |
| 1 | RA | 1962 | 5MC | C5-C4 | 5.58 | 1.50 | 1.41 |
| 1 | YA | 2605 | PSU | C2-N1 | 5.58 | 1.49 | 1.38 |
| 1 | RA | 1917 | PSU | C2-N3 | 5.58 | 1.49 | 1.38 |
| 32 | QA | 1407 | 5MC | C5-C4 | 5.59 | 1.50 | 1.41 |
| 1 | YA | 1911 | PSU | C2-N1 | 5.61 | 1.49 | 1.38 |
| 32 | XA | 1400 | 5MC | C5-C4 | 5.62 | 1.50 | 1.41 |
| 32 | XA | 1407 | 5MC | C5-C4 | 5.62 | 1.50 | 1.41 |
| 32 | QA | 1400 | 5MC | C5-C4 | 5.64 | 1.50 | 1.41 |
| 32 | QA | 1404 | 5MC | C5-C4 | 5.64 | 1.50 | 1.41 |
| 1 | YA | 1942 | 5MC | C5-C4 | 5.66 | 1.50 | 1.41 |
| 1 | RA | 2605 | PSU | C2-N1 | 5.67 | 1.50 | 1.38 |
| 32 | XA | 1404 | 5MC | C5-C4 | 5.68 | 1.50 | 1.41 |
| 1 | RA | 1911 | PSU | C2-N1 | 5.69 | 1.50 | 1.38 |
| 32 | XA | 516 | PSU | C2-N1 | 5.71 | 1.50 | 1.38 |
| 1 | RA | 2503 | 2MA | C2-N1 | 5.71 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 32 | XA | 967 | 5MC | C5-C4 | 5.71 | 1.50 | 1.41 |
| 1 | YA | 2503 | 2MA | C2-N1 | 5.72 | 1.44 | 1.34 |
| 1 | YA | 2251 | OMG | C6-N1 | 5.73 | 1.43 | 1.33 |
| 1 | RA | 1942 | 5MC | C5-C4 | 5.73 | 1.50 | 1.41 |
| 1 | YA | 1917 | PSU | C2-N1 | 5.75 | 1.50 | 1.38 |
| 1 | RA | 2251 | OMG | C6-N1 | 5.79 | 1.43 | 1.33 |
| 1 | YA | 2251 | OMG | C2-N1 | 5.80 | 1.46 | 1.35 |
| 32 | QA | 967 | 5MC | C5-C4 | 5.80 | 1.50 | 1.41 |
| 1 | YA | 1920 | 4OC | C4-N3 | 5.81 | 1.46 | 1.35 |
| 32 | QA | 516 | PSU | C2-N1 | 5.83 | 1.50 | 1.38 |
| 1 | RA | 2251 | OMG | C2-N1 | 5.83 | 1.46 | 1.35 |
| 1 | RA | 1920 | 4OC | C4-N3 | 5.84 | 1.46 | 1.35 |
| 1 | RA | 1917 | PSU | C2-N1 | 5.88 | 1.50 | 1.38 |
| 32 | XA | 1402 | 4OC | C4-N3 | 5.90 | 1.45 | 1.34 |
| 1 | YA | 2251 | OMG | C6-C5 | 6.08 | 1.53 | 1.41 |
| 1 | RA | 2251 | OMG | C6-C5 | 6.15 | 1.53 | 1.41 |
| 32 | QA | 966 | M2G | C2-N1 | 6.20 | 1.45 | 1.34 |
| 32 | XA | 1207 | 2MG | C6-N1 | 6.21 | 1.44 | 1.33 |
| 32 | QA | 1207 | 2MG | C6-C5 | 6.21 | 1.53 | 1.41 |
| 32 | QA | 1207 | 2MG | C6-N1 | 6.22 | 1.44 | 1.33 |
| 32 | XA | 966 | M2G | C2-N1 | 6.22 | 1.45 | 1.34 |
| 32 | XA | 1207 | 2MG | C6-C5 | 6.27 | 1.54 | 1.41 |
| 32 | QA | 1402 | 4OC | C4-N3 | 6.38 | 1.46 | 1.34 |
| 1 | RA | 1917 | PSU | C6-C5 | 6.43 | 1.47 | 1.38 |
| 1 | YA | 1911 | PSU | C6-C5 | 6.43 | 1.47 | 1.38 |
| 1 | YA | 1917 | PSU | C6-C5 | 6.44 | 1.47 | 1.38 |
| 32 | QA | 966 | M2G | C6-C5 | 6.46 | 1.54 | 1.41 |
| 32 | XA | 966 | M2G | C6-C5 | 6.53 | 1.54 | 1.41 |
| 1 | YA | 2605 | PSU | C6-C5 | 6.56 | 1.47 | 1.38 |
| 32 | XA | 516 | PSU | C6-C5 | 6.57 | 1.47 | 1.38 |
| 1 | RA | 1911 | PSU | C6-C5 | 6.57 | 1.47 | 1.38 |
| 1 | YA | 2503 | 2MA | C6-C5 | 6.62 | 1.53 | 1.40 |
| 32 | QA | 966 | M2G | C6-N1 | 6.63 | 1.45 | 1.33 |
| 32 | XA | 966 | M2G | C6-N1 | 6.63 | 1.45 | 1.33 |
| 32 | QA | 516 | PSU | C6-C5 | 6.74 | 1.48 | 1.38 |
| 1 | RA | 2605 | PSU | C6-C5 | 6.84 | 1.48 | 1.38 |
| 32 | XA | 527 | 7MG | C2-N3 | 6.86 | 1.48 | 1.35 |
| 1 | RA | 2503 | 2MA | C6-C5 | 6.87 | 1.53 | 1.40 |
| 32 | QA | 1498 | UR3 | C4-N3 | 6.87 | 1.48 | 1.38 |
| 32 | XA | 1498 | UR3 | C4-N3 | 6.94 | 1.48 | 1.38 |
| 32 | QA | 527 | 7MG | C2-N3 | 6.95 | 1.48 | 1.35 |
| 32 | XA | 1404 | 5MC | C4-N3 | 6.97 | 1.45 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1 | YA | 2251 | OMG | C4-N3 | 7.03 | 1.46 | 1.35 |
| 32 | QA | 1404 | 5MC | C4-N3 | 7.14 | 1.45 | 1.35 |
| 32 | QA | 527 | 7MG | C2-N1 | 7.14 | 1.48 | 1.35 |
| 32 | XA | 527 | 7MG | C2-N1 | 7.15 | 1.48 | 1.35 |
| 1 | RA | 2251 | OMG | C4-N3 | 7.17 | 1.47 | 1.35 |
| 32 | XA | 967 | 5MC | C4-N3 | 7.18 | 1.45 | 1.35 |
| 32 | QA | 1407 | 5MC | C4-N3 | 7.19 | 1.45 | 1.35 |
| 32 | QA | 1400 | 5MC | C4-N3 | 7.21 | 1.45 | 1.35 |
| 32 | XA | 1407 | 5MC | C4-N3 | 7.26 | 1.45 | 1.35 |
| 32 | XA | 1400 | 5MC | C4-N3 | 7.29 | 1.45 | 1.35 |
| 1 | RA | 1962 | 5MC | C4-N3 | 7.39 | 1.46 | 1.35 |
| 32 | QA | 967 | 5MC | C4-N3 | 7.42 | 1.46 | 1.35 |
| 1 | RA | 2503 | 2MA | C2-N3 | 7.44 | 1.47 | 1.34 |
| 1 | YA | 1942 | 5MC | C4-N3 | 7.45 | 1.46 | 1.35 |
| 1 | YA | 1962 | 5MC | C4-N3 | 7.52 | 1.46 | 1.35 |
| 1 | RA | 1942 | 5MC | C4-N3 | 7.53 | 1.46 | 1.35 |
| 1 | YA | 2503 | 2MA | C2-N3 | 7.56 | 1.48 | 1.34 |
| 32 | QA | 516 | PSU | C4-N3 | 7.56 | 1.46 | 1.33 |
| 32 | XA | 516 | PSU | C4-N3 | 7.60 | 1.46 | 1.33 |
| 1 | RA | 2605 | PSU | C4-N3 | 7.63 | 1.46 | 1.33 |
| 1 | YA | 1917 | PSU | C4-N3 | 7.68 | 1.46 | 1.33 |
| 1 | RA | 1917 | PSU | C4-N3 | 7.70 | 1.46 | 1.33 |
| 1 | YA | 1911 | PSU | C4-N3 | 7.75 | 1.47 | 1.33 |
| 1 | YA | 2605 | PSU | C4-N3 | 7.77 | 1.47 | 1.33 |
| 32 | QA | 527 | 7MG | C6-N1 | 7.81 | 1.47 | 1.33 |
| 1 | RA | 1911 | PSU | C4-N3 | 7.84 | 1.47 | 1.33 |
| 32 | XA | 527 | 7MG | C6-N1 | 7.94 | 1.47 | 1.33 |
| 1 | YA | 1920 | 4OC | C6-N1 | 7.95 | 1.46 | 1.35 |
| 1 | RA | 1920 | 4OC | C6-N1 | 7.97 | 1.46 | 1.35 |
| 32 | XA | 1402 | 4OC | C6-N1 | 8.00 | 1.46 | 1.35 |
| 32 | XA | 1207 | 2MG | C4-N3 | 8.03 | 1.48 | 1.35 |
| 32 | QA | 1402 | 4OC | C6-N1 | 8.13 | 1.46 | 1.35 |
| 32 | XA | 966 | M2G | C2-N2 | 8.16 | 1.48 | 1.34 |
| 32 | QA | 1207 | 2MG | C4-N3 | 8.23 | 1.48 | 1.35 |
| 32 | QA | 966 | M2G | C2-N2 | 8.38 | 1.49 | 1.34 |
| 32 | QA | 527 | 7MG | C6-C5 | 8.75 | 1.53 | 1.41 |
| 32 | XA | 966 | M2G | C4-N3 | 8.86 | 1.49 | 1.35 |
| 32 | XA | 527 | 7MG | C6-C5 | 8.87 | 1.54 | 1.41 |
| 32 | QA | 1498 | UR3 | C6-N1 | 9.03 | 1.47 | 1.35 |
| 32 | XA | 1498 | UR3 | C6-N1 | 9.17 | 1.47 | 1.35 |
| 32 | QA | 966 | M2G | C4-N3 | 9.18 | 1.50 | 1.35 |
| 32 | XA | 1207 | 2MG | C2-N2 | 9.38 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 32 | QA | 1207 | 2MG | C2-N2 | 9.42 | 1.45 | 1.34 |
| 1 | RA | 2503 | 2MA | C4-N3 | 10.14 | 1.51 | 1.35 |
| 1 | YA | 2503 | 2MA | C4-N3 | 10.48 | 1.52 | 1.35 |
| 32 | XA | 527 | 7MG | C4-N3 | 10.84 | 1.48 | 1.34 |
| 32 | QA | 527 | 7MG | C4-N3 | 10.94 | 1.48 | 1.34 |
| 1 | YA | 2552 | 2MU | O4'-C1' | 11.58 | 1.57 | 1.41 |
| 1 | RA | 2552 | 2MU | O4'-C1' | 11.63 | 1.57 | 1.41 |
| 1 | RA | 2552 | 2MU | C6-N1 | 23.02 | 1.65 | 1.35 |
| 1 | YA | 2552 | 2MU | C6-N1 | 23.06 | 1.65 | 1.35 |

All (141) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 32 | QA | 966 | M2G | C1'-N9-C4 | -12.99 | 112.31 | 126.81 |
| 1 | RA | 2503 | 2MA | C1'-N9-C4 | -11.96 | 113.46 | 126.81 |
| 1 | YA | 2503 | 2MA | C1'-N9-C4 | -11.95 | 113.47 | 126.81 |
| 32 | XA | 966 | M2G | C1'-N9-C4 | -11.61 | 113.85 | 126.81 |
| 32 | XA | 1402 | 4OC | CM4-N4-C4 | -11.59 | 113.10 | 122.87 |
| 32 | XA | 1519 | MA6 | N3-C2-N1 | -10.59 | 120.55 | 128.87 |
| 32 | QA | 1518 | MA6 | N3-C2-N1 | -10.25 | 120.82 | 128.87 |
| 32 | XA | 1518 | MA6 | N3-C2-N1 | -10.01 | 121.01 | 128.87 |
| 32 | QA | 1519 | MA6 | N3-C2-N1 | -9.37 | 121.51 | 128.87 |
| 32 | QA | 1402 | 4OC | CM4-N4-C4 | -6.70 | 117.22 | 122.87 |
| 1 | RA | 2251 | OMG | N3-C2-N1 | -6.61 | 118.57 | 127.56 |
| 1 | YA | 2251 | OMG | N3-C2-N1 | -6.54 | 118.66 | 127.56 |
| 32 | QA | 527 | 7MG | C5-C4-N3 | -5.96 | 120.67 | 126.74 |
| 32 | XA | 1207 | 2MG | CM2-N2-C2 | -5.58 | 116.76 | 123.03 |
| 32 | XA | 527 | 7MG | C5-C4-N3 | -5.57 | 121.06 | 126.74 |
| 32 | QA | 1207 | 2MG | CM2-N2-C2 | -5.42 | 116.94 | 123.03 |
| 32 | QA | 1207 | 2MG | N3-C2-N1 | -4.85 | 118.93 | 126.19 |
| 32 | XA | 527 | 7MG | N1-C2-N3 | -4.67 | 117.88 | 125.51 |
| 32 | XA | 1207 | 2MG | N3-C2-N1 | -4.61 | 119.29 | 126.19 |
| 43 | QL | 92 | 0TD | CB-CA-N | -4.57 | 100.68 | 109.83 |
| 32 | QA | 527 | 7MG | N1-C2-N3 | -4.28 | 118.52 | 125.51 |
| 43 | XL | 92 | 0TD | CB-CA-N | -4.02 | 101.78 | 109.83 |
| 32 | QA | 966 | M2G | N3-C2-N1 | -3.97 | 119.61 | 126.35 |
| 32 | XA | 966 | M2G | N3-C2-N1 | -3.72 | 120.03 | 126.35 |
| 1 | YA | 2503 | 2MA | N3-C2-N1 | -3.28 | 119.17 | 125.60 |
| 1 | RA | 2503 | 2MA | N3-C2-N1 | -3.22 | 119.29 | 125.60 |
| 32 | XA | 966 | M2G | CM1-N2-C2 | -3.19 | 118.13 | 121.34 |
| 32 | QA | 527 | 7MG | C5-C6-N1 | -3.13 | 118.73 | 123.39 |
| 1 | RA | 1917 | PSU | C5-C6-N1 | -3.06 | 120.12 | 124.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | RA | 2605 | PSU | C5-C6-N1 | -3.00 | 120.19 | 124.38 |
| 1 | YA | 2552 | 2MU | C4'-O4'-C1' | -2.97 | 106.50 | 109.64 |
| 1 | YA | 2605 | PSU | C5-C6-N1 | -2.96 | 120.26 | 124.38 |
| 32 | QA | 516 | PSU | C5-C6-N1 | -2.96 | 120.26 | 124.38 |
| 1 | YA | 2251 | OMG | C5-C6-N1 | -2.92 | 119.70 | 123.52 |
| 1 | RA | 2251 | OMG | C5-C6-N1 | -2.91 | 119.71 | 123.52 |
| 32 | XA | 527 | 7MG | C5-C6-N1 | -2.90 | 119.07 | 123.39 |
| 32 | XA | 966 | M2G | C5-C6-N1 | -2.86 | 119.79 | 123.52 |
| 32 | QA | 1207 | 2MG | C5-C6-N1 | -2.86 | 119.79 | 123.52 |
| 1 | YA | 1917 | PSU | C5-C6-N1 | -2.80 | 120.48 | 124.38 |
| 1 | RA | 2605 | PSU | C5-C1'-C2' | -2.79 | 110.70 | 115.44 |
| 1 | YA | 2605 | PSU | C5-C1'-C2' | -2.75 | 110.77 | 115.44 |
| 1 | YA | 1911 | PSU | C5-C6-N1 | -2.73 | 120.58 | 124.38 |
| 32 | XA | 1207 | 2MG | C5-C6-N1 | -2.71 | 119.98 | 123.52 |
| 32 | XA | 516 | PSU | C5-C6-N1 | -2.71 | 120.61 | 124.38 |
| 1 | RA | 1917 | PSU | C5-C1'-C2' | -2.63 | 110.97 | 115.44 |
| 1 | RA | 1911 | PSU | C5-C6-N1 | -2.58 | 120.79 | 124.38 |
| 32 | QA | 966 | M2G | C5-C6-N1 | -2.55 | 120.19 | 123.52 |
| 1 | YA | 1911 | PSU | C5-C1'-C2' | -2.53 | 111.14 | 115.44 |
| 1 | YA | 1917 | PSU | C5-C1'-C2' | -2.50 | 111.20 | 115.44 |
| 55 | QY | 235 | MEQ | CB-CG-CD | -2.45 | 107.66 | 113.26 |
| 1 | RA | 2552 | 2MU | C4'-O4'-C1' | -2.31 | 107.20 | 109.64 |
| 32 | XA | 1519 | MA6 | C1'-N9-C4 | -2.27 | 124.27 | 126.81 |
| 32 | QA | 1404 | 5MC | CM5-C5-C4 | -2.20 | 119.14 | 121.47 |
| 1 | YA | 2251 | OMG | C6-C5-C4 | -2.19 | 118.35 | 120.86 |
| 32 | QA | 966 | M2G | CM2-N2-C2 | -2.19 | 119.14 | 121.34 |
| 1 | RA | 1920 | 4OC | C5-C4-N3 | -2.10 | 119.14 | 121.79 |
| 1 | YA | 1920 | 4OC | C5-C4-N3 | -2.06 | 119.18 | 121.79 |
| 1 | RA | 2251 | OMG | C6-C5-C4 | -2.05 | 118.52 | 120.86 |
| 32 | XA | 1404 | 5MC | CM5-C5-C4 | -2.00 | 119.35 | 121.47 |
| 32 | QA | 527 | 7MG | N2-C2-N3 | 2.01 | 120.52 | 117.20 |
| 1 | RA | 1962 | 5MC | N4-C4-N3 | 2.04 | 119.91 | 116.92 |
| 32 | QA | 967 | 5MC | N4-C4-N3 | 2.05 | 119.93 | 116.92 |
| 1 | RA | 1942 | 5MC | N4-C4-N3 | 2.06 | 119.94 | 116.92 |
| 32 | XA | 967 | 5MC | N4-C4-N3 | 2.07 | 119.95 | 116.92 |
| 32 | XA | 527 | 7MG | N3-C4-N9 | 2.08 | 129.67 | 126.98 |
| 32 | XA | 527 | 7MG | N2-C2-N3 | 2.09 | 120.65 | 117.20 |
| 32 | QA | 1404 | 5MC | N4-C4-N3 | 2.10 | 120.00 | 116.92 |
| 32 | QA | 1407 | 5MC | N4-C4-N3 | 2.11 | 120.01 | 116.92 |
| 32 | XA | 1407 | 5MC | N4-C4-N3 | 2.13 | 120.04 | 116.92 |
| 32 | QA | 1207 | 2MG | O3'-C3'-C2' | 2.20 | 118.96 | 111.86 |
| 1 | YA | 1939 | 5MU | C5-C4-N3 | 2.20 | 127.19 | 125.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 32 | XA | 1400 | 5MC | N4-C4-N3 | 2.20 | 120.15 | 116.92 |
| 1 | YA | 1942 | 5MC | N4-C4-N3 | 2.26 | 120.23 | 116.92 |
| 32 | QA | 527 | 7MG | N2-C2-N1 | 2.28 | 120.97 | 117.20 |
| 32 | QA | 527 | 7MG | C2-N3-C4 | 2.31 | 121.08 | 114.50 |
| 1 | RA | 2503 | 2MA | CM2-C2-N3 | 2.34 | 121.20 | 117.22 |
| 1 | YA | 1962 | 5MC | N4-C4-N3 | 2.35 | 120.37 | 116.92 |
| 1 | RA | 2605 | PSU | O4'-C1'-C2' | 2.42 | 107.30 | 104.69 |
| 1 | YA | 1915 | 5MU | C5-C4-N3 | 2.44 | 127.39 | 125.35 |
| 32 | XA | 527 | 7MG | C2-N3-C4 | 2.47 | 121.52 | 114.50 |
| 1 | YA | 2605 | PSU | O4'-C1'-C2' | 2.47 | 107.36 | 104.69 |
| 1 | YA | 2503 | 2MA | CM2-C2-N3 | 2.49 | 121.46 | 117.22 |
| 1 | RA | 2251 | OMG | N2-C2-N1 | 2.51 | 121.34 | 117.20 |
| 1 | YA | 2251 | OMG | N2-C2-N1 | 2.52 | 121.35 | 117.20 |
| 1 | RA | 1911 | PSU | O4'-C1'-C2' | 2.52 | 107.41 | 104.69 |
| 32 | QA | 527 | 7MG | N3-C4-N9 | 2.53 | 130.26 | 126.98 |
| 1 | RA | 1939 | 5MU | C5M-C5-C4 | 2.55 | 122.79 | 119.97 |
| 32 | XA | 527 | 7MG | N2-C2-N1 | 2.59 | 121.47 | 117.20 |
| 1 | YA | 1911 | PSU | O4'-C1'-C2' | 2.62 | 107.52 | 104.69 |
| 32 | QA | 966 | M2G | N1-C2-N2 | 2.62 | 119.99 | 117.14 |
| 1 | YA | 1917 | PSU | O4'-C1'-C2' | 2.63 | 107.53 | 104.69 |
| 1 | RA | 1915 | 5MU | C5M-C5-C4 | 2.71 | 122.97 | 119.97 |
| 1 | RA | 1917 | PSU | O4'-C1'-C2' | 2.73 | 107.64 | 104.69 |
| 1 | YA | 1915 | 5MU | C5M-C5-C4 | 2.90 | 123.18 | 119.97 |
| 32 | QA | 966 | M2G | N3-C2-N2 | 2.96 | 120.40 | 117.14 |
| 43 | QL | 92 | 0TD | CSB-SB-CB | 3.03 | 107.10 | 101.44 |
| 32 | XA | 516 | PSU | O4'-C1'-C2' | 3.10 | 108.04 | 104.69 |
| 32 | QA | 516 | PSU | O4'-C1'-C2' | 3.10 | 108.04 | 104.69 |
| 32 | QA | 1519 | MA6 | C2-N1-C6 | 3.30 | 119.42 | 111.64 |
| 43 | XL | 92 | 0TD | CSB-SB-CB | 3.31 | 107.64 | 101.44 |
| 32 | XA | 1207 | 2MG | C6-N1-C2 | 3.34 | 120.02 | 115.24 |
| 1 | YA | 1939 | 5MU | C5M-C5-C4 | 3.57 | 123.92 | 119.97 |
| 1 | RA | 2552 | 2MU | C4-N3-C2 | 3.60 | 118.00 | 114.21 |
| 32 | XA | 1402 | 4OC | C6-C5-C4 | 3.63 | 118.85 | 117.42 |
| 1 | YA | 2552 | 2MU | C4-N3-C2 | 3.64 | 118.05 | 114.21 |
| 32 | QA | 1518 | MA6 | C2-N1-C6 | 3.65 | 120.26 | 111.64 |
| 32 | QA | 1207 | 2MG | C6-N1-C2 | 3.69 | 120.52 | 115.24 |
| 32 | XA | 1518 | MA6 | C2-N1-C6 | 3.70 | 120.37 | 111.64 |
| 32 | XA | 1519 | MA6 | C2-N1-C6 | 3.73 | 120.44 | 111.64 |
| 32 | QA | 1402 | 4OC | C6-C5-C4 | 3.75 | 118.89 | 117.42 |
| 32 | XA | 1402 | 4OC | C2-N3-C4 | 3.96 | 120.47 | 115.43 |
| 1 | RA | 2251 | OMG | C6-N1-C2 | 4.12 | 120.71 | 115.88 |
| 1 | YA | 2251 | OMG | C6-N1-C2 | 4.13 | 120.72 | 115.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 32 | XA | 966 | M2G | N1-C2-N2 | 4.31 | 121.84 | 117.14 |
| 32 | QA | 1402 | 4OC | C2-N3-C4 | 4.37 | 120.99 | 115.43 |
| 32 | XA | 1207 | 2MG | N2-C2-N1 | 4.70 | 122.40 | 116.94 |
| 32 | QA | 1207 | 2MG | N2-C2-N1 | 4.73 | 122.43 | 116.94 |
| 32 | QA | 527 | 7MG | C6-N1-C2 | 4.98 | 121.72 | 115.88 |
| 1 | YA | 2605 | PSU | C4-N3-C2 | 5.03 | 119.35 | 115.16 |
| 32 | QA | 1207 | 2MG | C2-N3-C4 | 5.04 | 120.52 | 114.99 |
| 1 | RA | 1915 | 5MU | C4-N3-C2 | 5.08 | 119.40 | 115.16 |
| 32 | XA | 527 | 7MG | C6-N1-C2 | 5.09 | 121.84 | 115.88 |
| 32 | XA | 1207 | 2MG | C2-N3-C4 | 5.15 | 120.64 | 114.99 |
| 1 | RA | 2605 | PSU | C4-N3-C2 | 5.17 | 119.47 | 115.16 |
| 1 | YA | 1915 | 5MU | C4-N3-C2 | 5.19 | 119.49 | 115.16 |
| 1 | YA | 1939 | 5MU | C4-N3-C2 | 5.39 | 119.66 | 115.16 |
| 32 | QA | 966 | M2G | C2-N3-C4 | 5.50 | 121.02 | 114.99 |
| 32 | XA | 966 | M2G | C2-N3-C4 | 5.53 | 121.06 | 114.99 |
| 32 | QA | 516 | PSU | C4-N3-C2 | 5.57 | 119.80 | 115.16 |
| 1 | RA | 1939 | 5MU | C4-N3-C2 | 5.59 | 119.82 | 115.16 |
| 1 | RA | 1920 | 4OC | C6-C5-C4 | 5.84 | 119.72 | 117.44 |
| 32 | XA | 516 | PSU | C4-N3-C2 | 5.96 | 120.13 | 115.16 |
| 1 | YA | 1917 | PSU | C4-N3-C2 | 6.03 | 120.19 | 115.16 |
| 1 | YA | 1911 | PSU | C4-N3-C2 | 6.16 | 120.30 | 115.16 |
| 1 | RA | 1911 | PSU | C4-N3-C2 | 6.17 | 120.30 | 115.16 |
| 1 | YA | 1920 | 4OC | C6-C5-C4 | 6.19 | 119.86 | 117.44 |
| 1 | RA | 1917 | PSU | C4-N3-C2 | 6.21 | 120.34 | 115.16 |
| 1 | YA | 2251 | OMG | C1'-N9-C4 | 6.87 | 134.48 | 126.81 |
| 1 | RA | 2251 | OMG | C1'-N9-C4 | 7.21 | 134.85 | 126.81 |
| 1 | YA | 2503 | 2MA | C2-N3-C4 | 13.67 | 121.88 | 115.29 |
| 1 | RA | 2503 | 2MA | C2-N3-C4 | 13.97 | 122.02 | 115.29 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 33 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32 | QA | 1402 | 4OC | 2 | 0 |
| 32 | QA | 1518 | MA6 | 1 | 0 |
| 32 | QA | 1519 | MA6 | 3 | 0 |
| 32 | QA | 966 | M2G | 1 | 0 |
| 1 | RA | 1917 | PSU | 1 | 0 |
| 1 | RA | 1939 | 5MU | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | RA | 1942 | 5MC | 1 | 0 |
| 1 | RA | 1962 | 5MC | 1 | 0 |
| 1 | RA | 2503 | 2MA | 2 | 0 |
| 1 | RA | 2552 | 2MU | 4 | 0 |
| 32 | XA | 1207 | 2MG | 1 | 0 |
| 32 | XA | 1402 | 4OC | 3 | 0 |
| 32 | XA | 1518 | MA6 | 2 | 0 |
| 32 | XA | 1519 | MA6 | 1 | 0 |
| 43 | XL | 92 | 0TD | 1 | 0 |
| 1 | YA | 1917 | PSU | 1 | 0 |
| 1 | YA | 1939 | 5MU | 1 | 0 |
| 1 | YA | 1942 | 5MC | 1 | 0 |
| 1 | YA | 1962 | 5MC | 1 | 0 |
| 1 | YA | 2503 | 2MA | 2 | 0 |
| 1 | YA | 2552 | 2MU | 4 | 0 |

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2445 ligands modelled in this entry, 2443 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 | $\# Z > 2$ |
| 58 | SF4 | QD | 302 | 35 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 58 | SF4 | XD | 301 | - | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 58 | SF4 | QD | 302 | 35 | - | 0/0/48/48 | 0/6/5/5 |
| 58 | SF4 | XD | 301 | - | - | 0/0/48/48 | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.