



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 08:14 pm BST

PDB ID : 6BZ7
Title : Thermus thermophilus 70S containing 16S G299A point mutation and near-cognate ASL Leucine in A site.
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.68 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

<https://www.wwpdb.org/validation/2017/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 | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

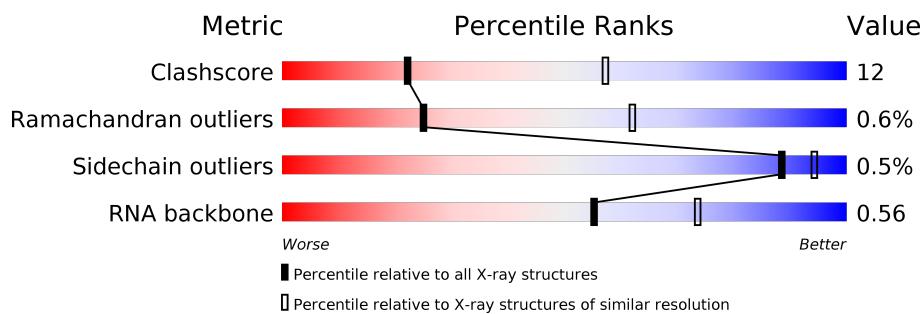
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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 | 141614 | 1070 (3.84-3.52) |
| Ramachandran outliers | 138981 | 1036 (3.84-3.52) |
| Sidechain outliers | 138945 | 1033 (3.84-3.52) |
| RNA backbone | 3102 | 1024 (4.30-3.00) |


























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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | QA | 1508 | 45% 44% 10% .. |
| 1 | XA | 1508 | 44% 45% 10% . |
| 2 | QB | 256 | 61% 30% . 8% |
| 2 | XB | 256 | 63% 28% . 8% |
| 3 | QC | 239 | 65% 21% 14% |
| 3 | XC | 239 | 66% 20% 14% |
| 4 | QD | 209 | 68% 31% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | XD | 209 |  |
| 5 | QE | 162 |  |
| 5 | XE | 162 |  |
| 6 | QF | 101 |  |
| 6 | XF | 101 |  |
| 7 | QG | 156 |  |
| 7 | XG | 156 |  |
| 8 | QH | 138 |  |
| 8 | XH | 138 |  |
| 9 | QI | 128 |  |
| 9 | XI | 128 |  |
| 10 | QJ | 105 |  |
| 10 | XJ | 105 |  |
| 11 | QK | 129 |  |
| 11 | XK | 129 |  |
| 12 | QL | 132 |  |
| 12 | XL | 132 |  |
| 13 | QM | 126 |  |
| 13 | XM | 126 |  |
| 14 | QN | 61 |  |
| 14 | XN | 61 |  |
| 15 | QO | 89 |  |
| 15 | XO | 89 |  |
| 16 | QP | 88 |  |
| 16 | XP | 88 |  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 17 | QQ | 105 | |
| 17 | XQ | 105 | |
| 18 | QR | 88 | |
| 18 | XR | 88 | |
| 19 | QS | 93 | |
| 19 | XS | 93 | |
| 20 | QT | 106 | |
| 20 | XT | 106 | |
| 21 | QU | 27 | |
| 21 | XU | 27 | |
| 22 | QV | 77 | |
| 22 | QW | 77 | |
| 22 | XV | 77 | |
| 22 | XW | 77 | |
| 23 | QX | 25 | |
| 23 | XX | 25 | |
| 24 | QY | 17 | |
| 24 | XY | 17 | |
| 25 | RA | 2915 | |
| 25 | YA | 2915 | |
| 26 | RB | 122 | |
| 26 | YB | 122 | |
| 27 | RD | 276 | |
| 27 | YD | 276 | |
| 28 | RE | 206 | |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | YE | 206 |  |
| 29 | RF | 210 |  |
| 29 | YF | 210 |  |
| 30 | RG | 182 |  |
| 30 | YG | 182 |  |
| 31 | RH | 180 |  |
| 31 | YH | 180 |  |
| 32 | RI | 148 |  |
| 32 | YI | 148 |  |
| 33 | RN | 140 |  |
| 33 | YN | 140 |  |
| 34 | RO | 122 |  |
| 34 | YO | 122 |  |
| 35 | RP | 150 |  |
| 35 | YP | 150 |  |
| 36 | RQ | 141 |  |
| 36 | YQ | 141 |  |
| 37 | RR | 118 |  |
| 37 | YR | 118 |  |
| 38 | RS | 112 |  |
| 38 | YS | 112 |  |
| 39 | RT | 146 |  |
| 39 | YT | 146 |  |
| 40 | RU | 118 |  |
| 40 | YU | 118 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 41 | RV | 101 |  |
| 41 | YV | 101 |  |
| 42 | RW | 113 |  |
| 42 | YW | 113 |  |
| 43 | RX | 96 |  |
| 43 | YX | 96 |  |
| 44 | RY | 110 |  |
| 44 | YY | 110 |  |
| 45 | RZ | 206 |  |
| 45 | YZ | 206 |  |
| 46 | R0 | 85 |  |
| 46 | Y0 | 85 |  |
| 47 | R1 | 98 |  |
| 47 | Y1 | 98 |  |
| 48 | R2 | 72 |  |
| 48 | Y2 | 72 |  |
| 49 | R3 | 60 |  |
| 49 | Y3 | 60 |  |
| 50 | R4 | 71 |  |
| 50 | Y4 | 71 |  |
| 51 | R5 | 60 |  |
| 51 | Y5 | 60 |  |
| 52 | R6 | 54 |  |
| 52 | Y6 | 54 |  |
| 53 | R7 | 49 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 53 | Y7 | 49 | <div><div></div><div>71%27%</div><div></div></div> |
| 54 | R8 | 65 | <div><div></div><div>65%31%</div><div></div></div> |
| 54 | Y8 | 65 | <div><div></div><div>69%26%</div><div></div></div> |
| 55 | R9 | 37 | <div><div></div><div>38%62%</div><div></div></div> |
| 55 | Y9 | 37 | <div><div></div><div>24%62%14%</div><div></div></div> |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 295575 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 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | QA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32246 | 14353 | 5981 | 10413 | 1499 | | | |
| 1 | XA | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32248 | 14354 | 5984 | 10411 | 1499 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|-------------|
| QA | 299 | A | G | engineered mutation | GB 55771382 |
| XA | 299 | A | G | engineered mutation | GB 55771382 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | QB | 235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1907 | 1217 | 342 | 343 | 5 | | | |
| 2 | XB | 236 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1223 | 343 | 344 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | QC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |
| 3 | XC | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1605 | 1011 | 313 | 280 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | QD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | XD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | QE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 5 | XE | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | QF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | XF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | QG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | XG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | QH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1108 | 700 | 214 | 192 | 2 | | | |
| 8 | XH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1108 | 700 | 214 | 192 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | QI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |
| 9 | XI | 126 | Total | C | N | O | 0 | 0 | 0 |
| | | | 998 | 633 | 193 | 172 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | QJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 801 | 504 | 157 | 139 | 1 | | | |
| 10 | XJ | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 777 | 487 | 153 | 136 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | QK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |
| 11 | XK | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 864 | 537 | 164 | 160 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | QL | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 975 | 614 | 196 | 164 | 1 | | | |
| 12 | XL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 956 | 603 | 193 | 159 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | QM | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 591 | 197 | 165 | 2 | | | |
| 13 | XM | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 946 | 585 | 195 | 164 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | QN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | XN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | QO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | XO | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 146 | 124 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | QP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |
| 16 | XP | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 705 | 446 | 140 | 118 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | QQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |
| 17 | XQ | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 834 | 534 | 155 | 143 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | QR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 18 | XR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | QS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 424 | 124 | 115 | 2 | | | |
| 19 | XS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 674 | 430 | 126 | 116 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | QT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | XT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | QU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |
| 21 | XU | 25 | Total | C | N | O | 0 | 0 | 0 |
| | | | 217 | 134 | 52 | 31 | | | |

- Molecule 22 is a RNA chain called tRNA fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | QV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 22 | QW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1618 | 722 | 292 | 529 | 75 | | | |
| 22 | XV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 22 | XW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1618 | 722 | 292 | 529 | 75 | | | |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23 | QX | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 169 | 76 | 29 | 56 | 8 | | | |
| 23 | XX | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 210 | 96 | 39 | 66 | 9 | | | |

- Molecule 24 is a RNA chain called ASL Leu.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 24 | QY | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 358 | 162 | 64 | 116 | 16 | | | |
| 24 | XY | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 358 | 162 | 64 | 116 | 16 | | | |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25 | RA | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62071 | 27627 | 11611 | 19952 | 2881 | | | |
| 25 | YA | 2883 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62091 | 27636 | 11613 | 19960 | 2882 | | | |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26 | RB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |
| 26 | YB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | RD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |
| 27 | YD | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2115 | 1335 | 420 | 357 | 3 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | RE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |
| 28 | YE | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29 | RF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |
| 29 | YF | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | RG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | YG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | RH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1336 | 848 | 251 | 236 | 1 | | | |
| 31 | YH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1336 | 848 | 251 | 236 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | RI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |
| 32 | YI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | RN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |
| 33 | YN | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | RO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 34 | YO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | RP | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 35 | YP | 147 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 698 | 229 | 192 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | RQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 36 | YQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 37 | RR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 37 | YR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 38 | RS | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |
| 38 | YS | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | RT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |
| 39 | YT | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | RU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 40 | YU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | RV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 41 | YV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | RW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |
| 42 | YW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43 | RX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |
| 43 | YX | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | RY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 525 | 155 | 132 | 6 | | | |
| 44 | YY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 818 | 525 | 155 | 132 | 6 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | RZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |
| 45 | YZ | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | R0 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 643 | 398 | 137 | 107 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | Y0 | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 599 | 370 | 127 | 101 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | R1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |
| 47 | Y1 | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 457 | 145 | 126 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | R2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |
| 48 | Y2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49 | R3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 49 | Y3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | R4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 565 | 356 | 103 | 101 | 5 | | | |
| 50 | Y4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 565 | 356 | 103 | 101 | 5 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | R5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 51 | Y5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | R6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 52 | Y6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53 | R7 | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 409 | 251 | 102 | 54 | 2 | | | |
| 53 | Y7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | R8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 54 | Y8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55 | R9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 55 | Y9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | QA | 68 | Total | Mg | 0 | 0 |
| | | | 68 | 68 | | |
| 56 | RP | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | YA | 546 | Total | Mg | 0 | 0 |
| | | | 546 | 546 | | |
| 56 | RT | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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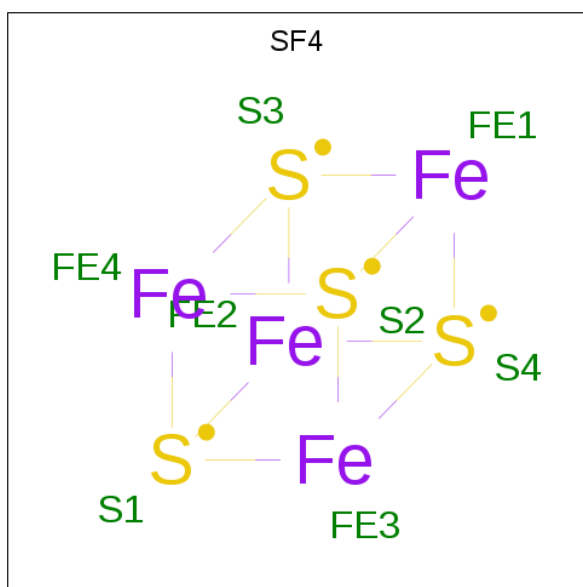
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56 | RN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XS | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | QV | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | Y8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XA | 82 | Total 82 | Mg 82 | 0 | 0 |
| 56 | YY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | R0 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | RU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | R4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YQ | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | RY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | R8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | RR | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | R1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | Y7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | Y0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RA | 508 | Total 508 | Mg 508 | 0 | 0 |
| 56 | YP | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | R9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RE | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | XL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YB | 12 | Total 12 | Mg 12 | 0 | 0 |
| 56 | QY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XV | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | RB | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | QE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XM | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | YE | 2 | Total 2 | Mg 2 | 0 | 0 |

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 57 | QD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 57 | XD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58 | Y9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | YY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | Y6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | QN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | XN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | RY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | Y4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | R6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | Y5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | R5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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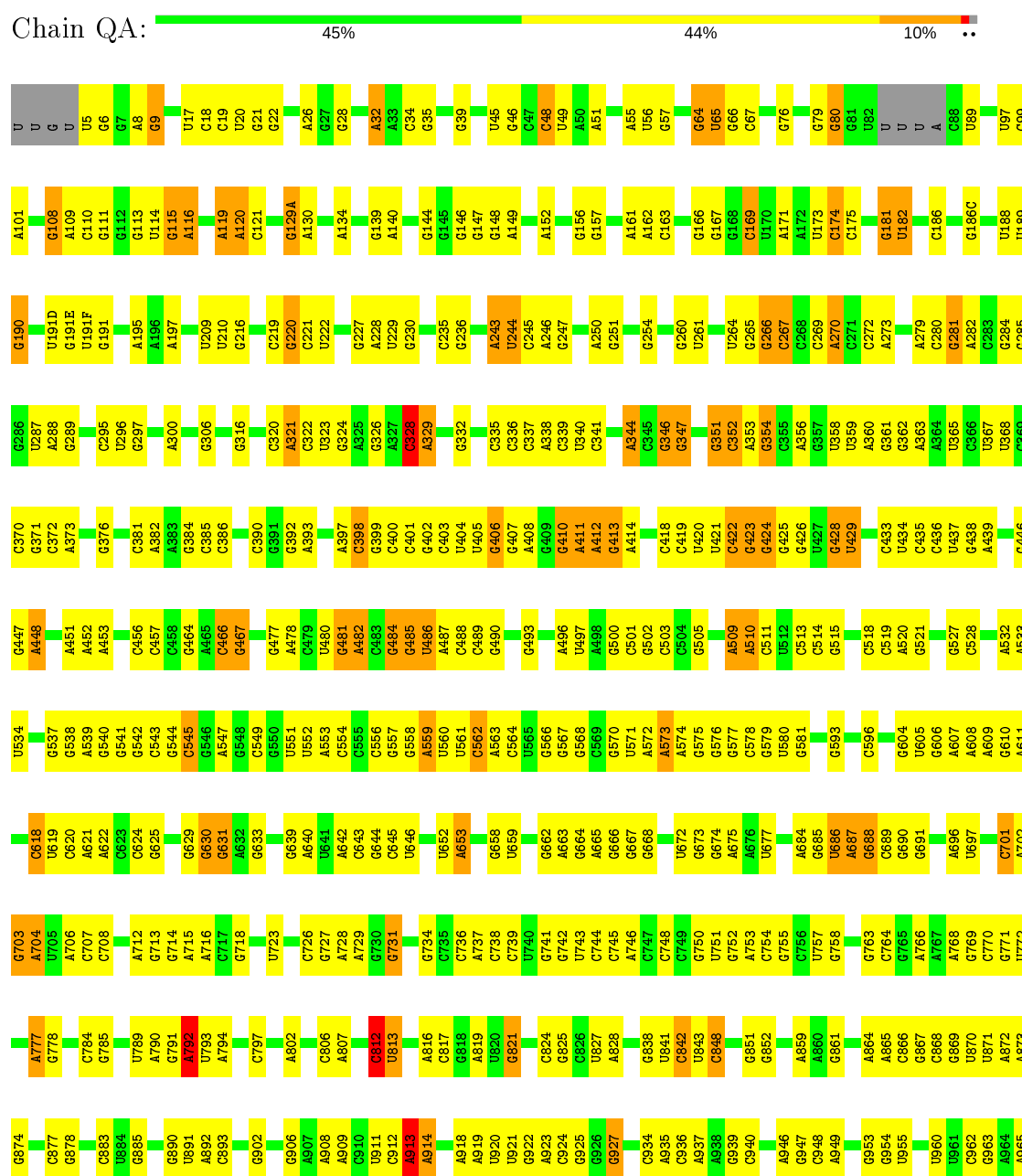
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 58 | R4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 58 | R9 | 1 | Total 1 | Zn 1 | 0 | 0 |

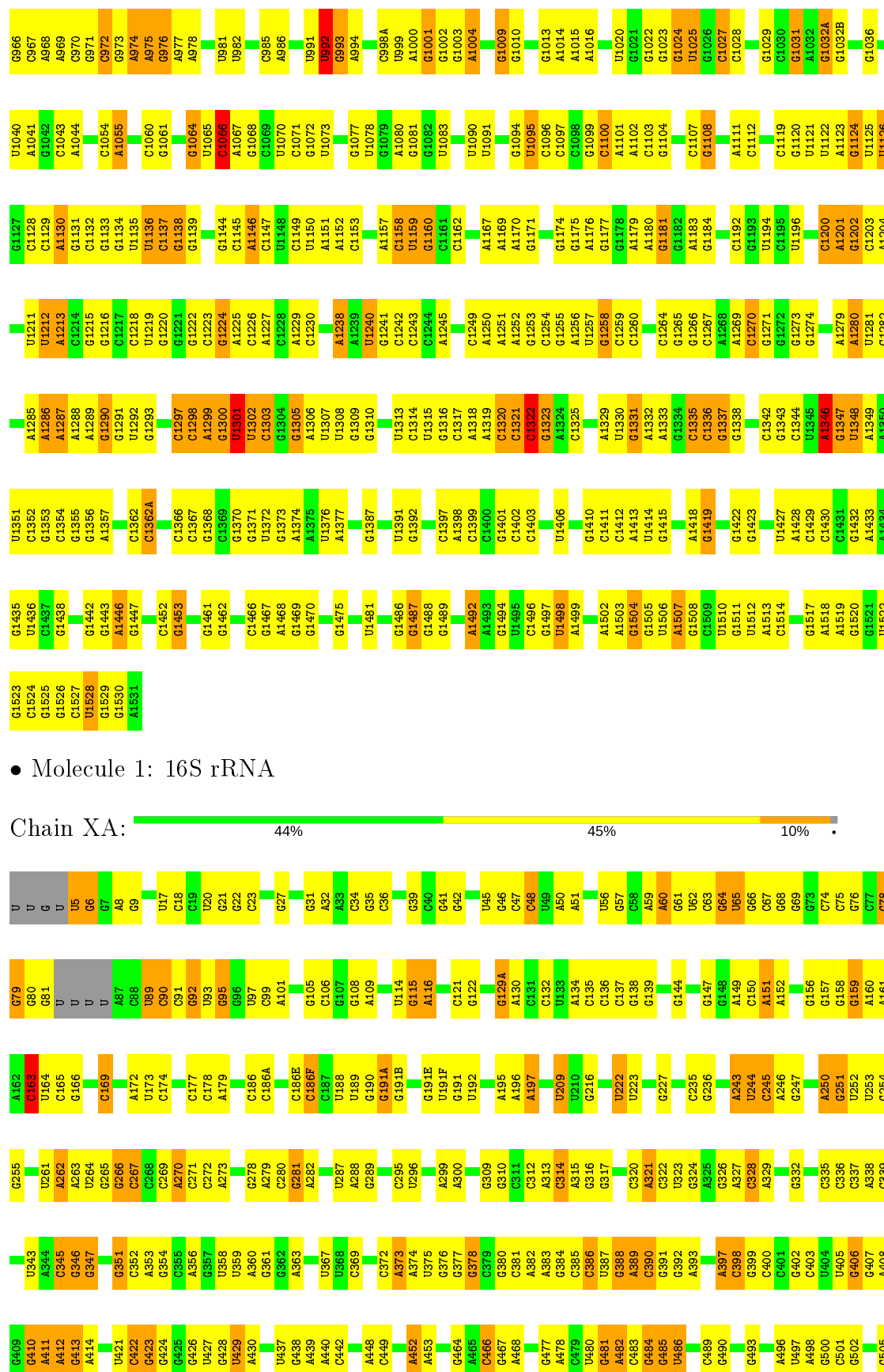
3 Residue-property plots

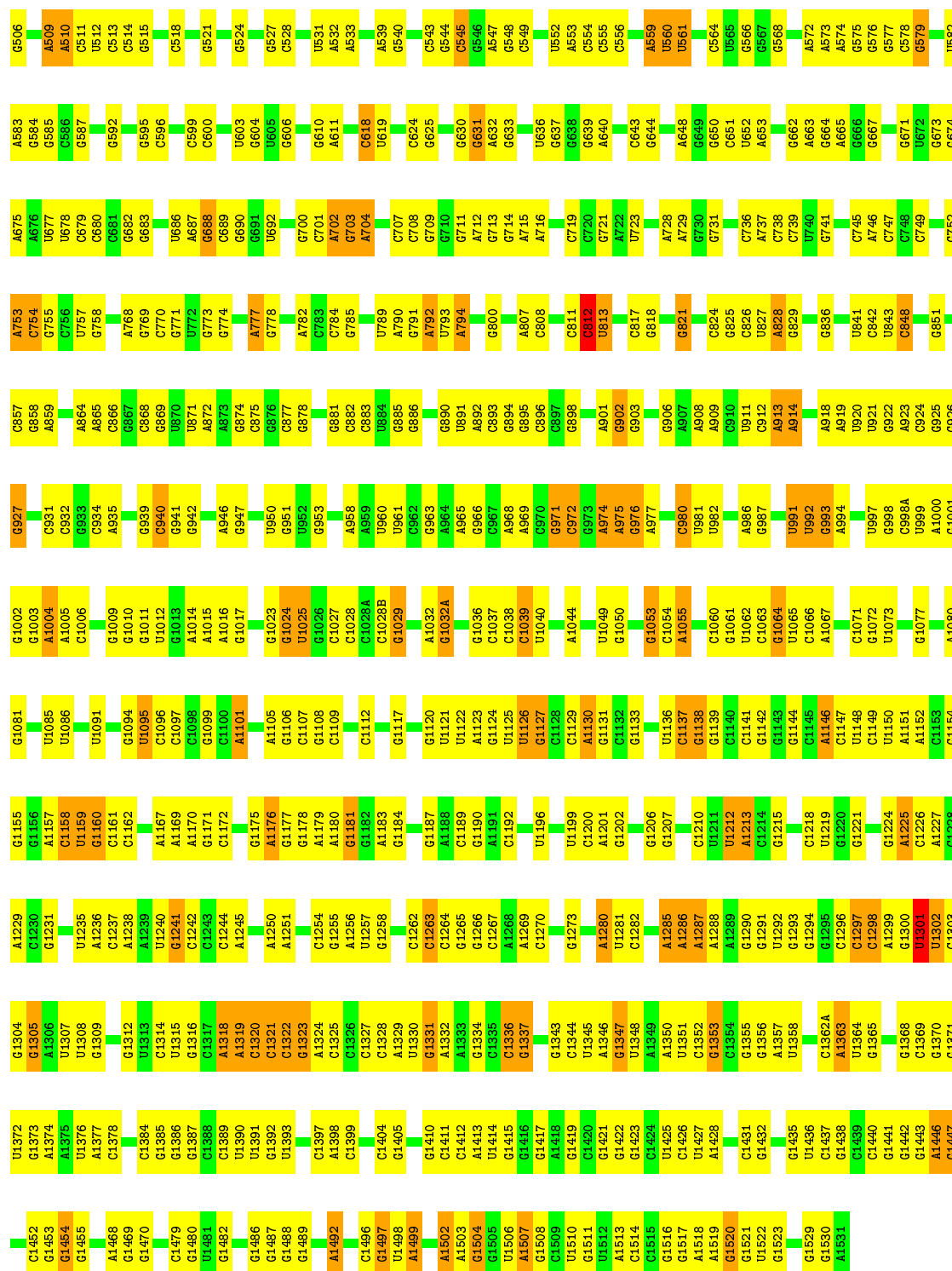
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS failed to run properly.

• Molecule 1: 16S rRNA



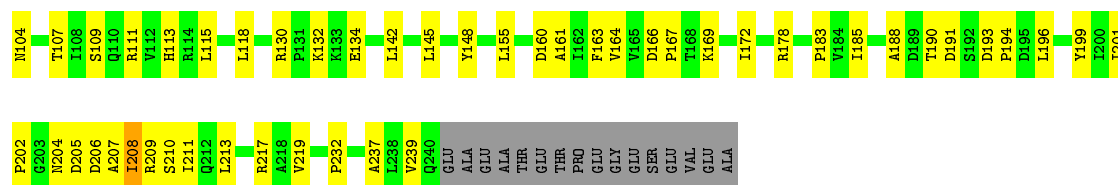




• Molecule 2: 30S ribosomal protein S2

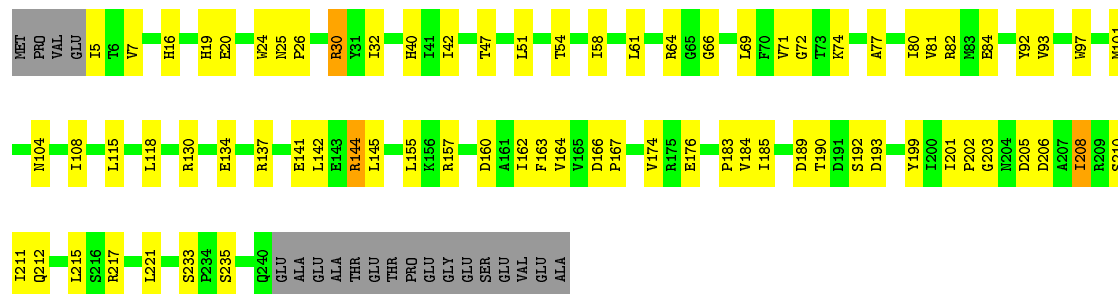
Chain QB:





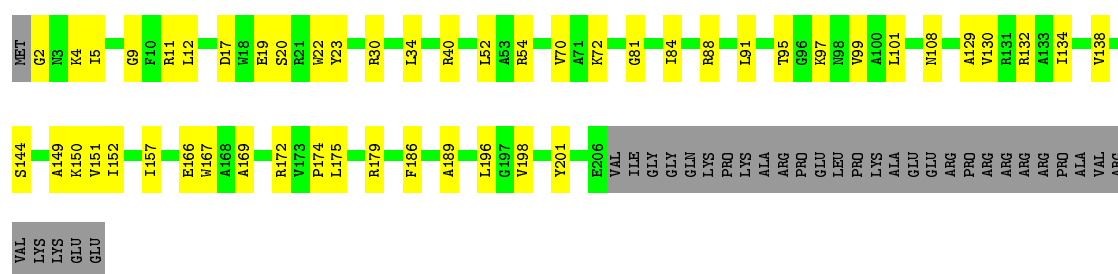
- Molecule 2: 30S ribosomal protein S2

Chain XB: 63% 28% 8%



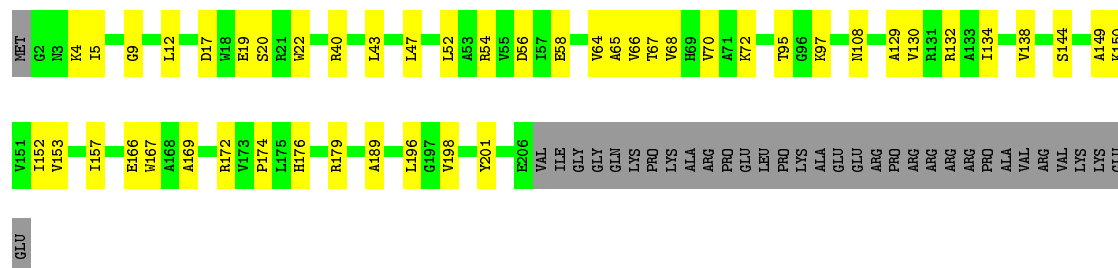
- Molecule 3: 30S ribosomal protein S3

Chain QC: 



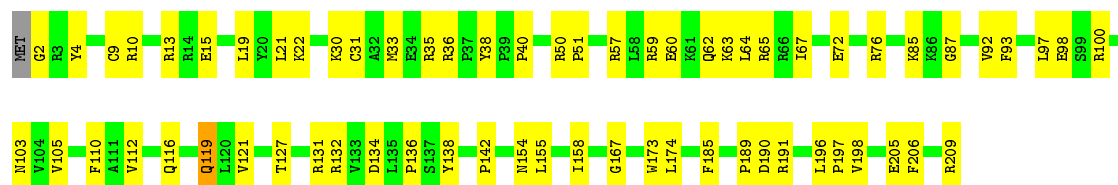
- Molecule 3: 30S ribosomal protein S3

Chain XC: 



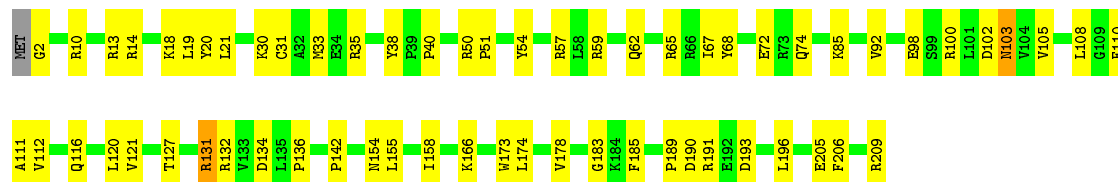
- Molecule 4: 30S ribosomal protein S4

Chain QD: 



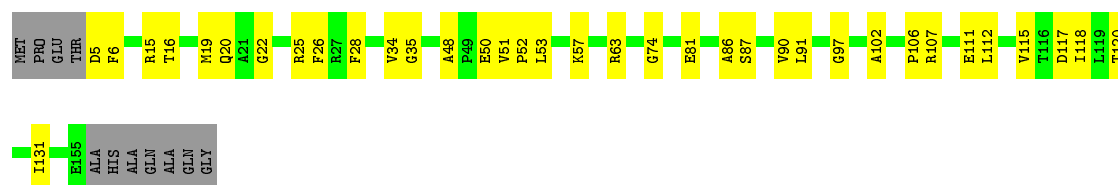
- Molecule 4: 30S ribosomal protein S4

Chain XD: 70% 29% .



- Molecule 5: 30S ribosomal protein S5

Chain QE: 71% 22% 7%



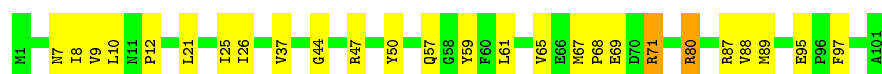
- Molecule 5: 30S ribosomal protein S5

Chain XE: 77% 17% 7%



- Molecule 6: 30S ribosomal protein S6

Chain QF: 74% 24%




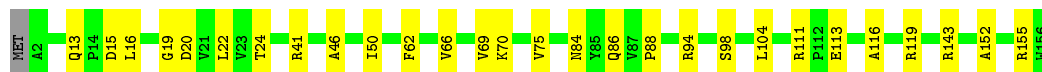
- Molecule 6: 30S ribosomal protein S6

Chain XF: 68% 32%




- Molecule 7: 30S ribosomal protein S7

Chain QG:  81% 18%




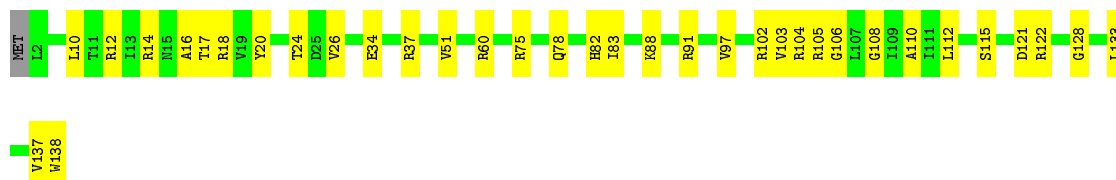
- Molecule 7: 30S ribosomal protein S7

Chain XG:  83% 16%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  74% 25%



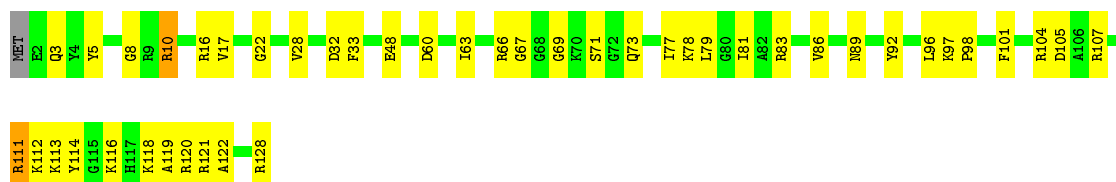
- Molecule 8: 30S ribosomal protein S8

Chain XH:  80% 20%



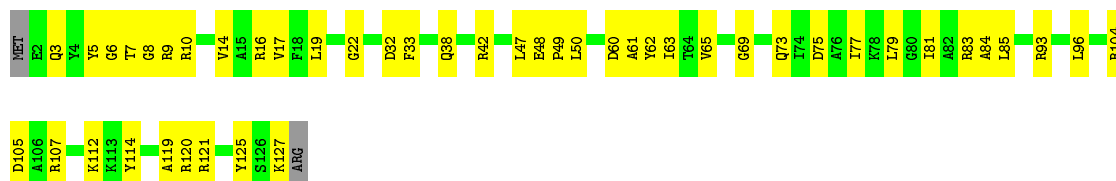
- Molecule 9: 30S ribosomal protein S9

Chain QI:  65% 33%



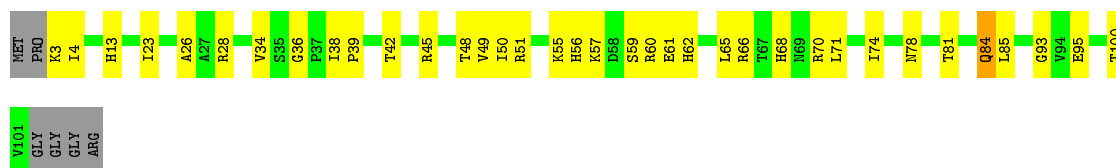
- Molecule 9: 30S ribosomal protein S9

Chain XI:  63% 36%



- Molecule 10: 30S ribosomal protein S10

Chain QJ: 



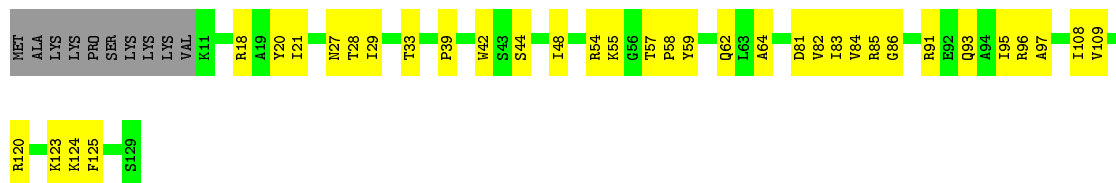
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 



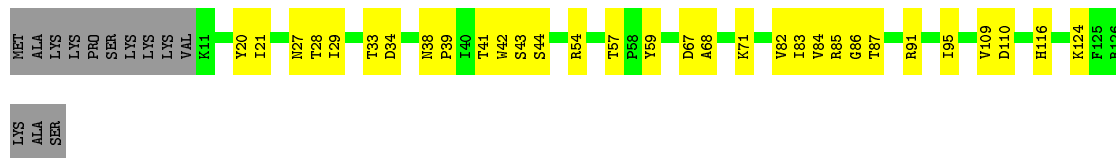
- Molecule 11: 30S ribosomal protein S11

Chain QK: 



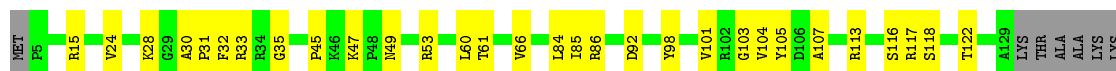
- Molecule 11: 30S ribosomal protein S11

Chain XK: 



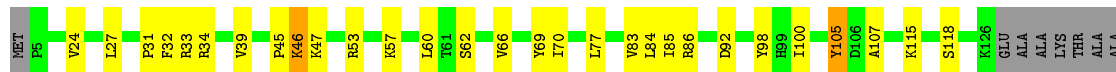
- Molecule 12: 30S ribosomal protein S12

Chain QL: 



- Molecule 12: 30S ribosomal protein S12

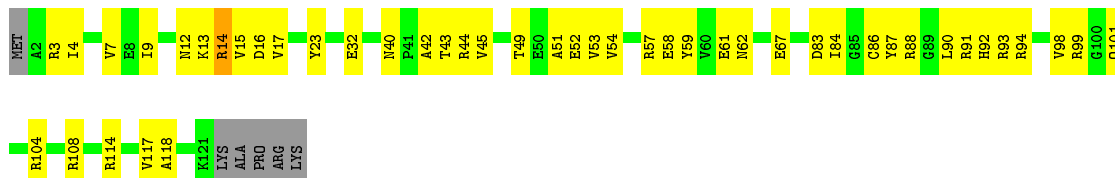
Chain XL: 



LYS
LYS

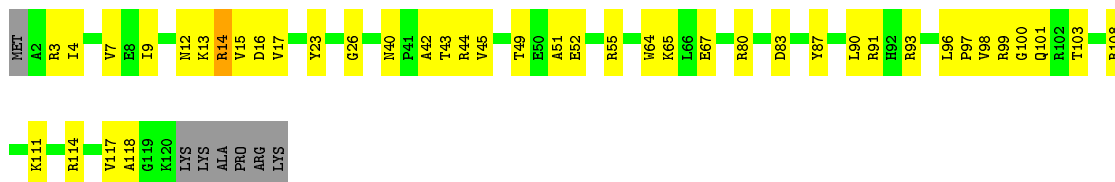
- Molecule 13: 30S ribosomal protein S13

Chain QM:  59% 36% • 5%



- Molecule 13: 30S ribosomal protein S13

Chain XM:  61% 33% • 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  72% 25% • •




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  72% 25% • •



- Molecule 15: 30S ribosomal protein S15

Chain QO:  80% 19% •

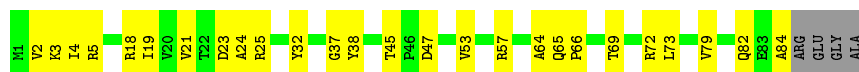


- Molecule 15: 30S ribosomal protein S15

Chain XO:  72% 26% •



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

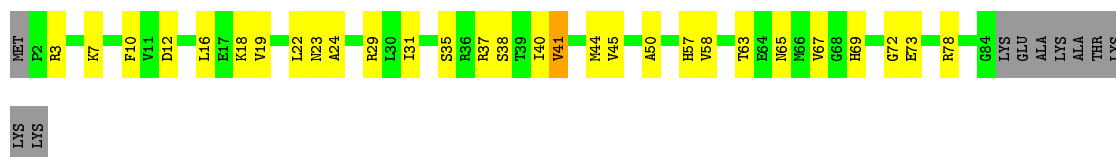


- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19





- Molecule 19: 30S ribosomal protein S19

Chain XS: 65% 25% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT: 69% 25% 7%



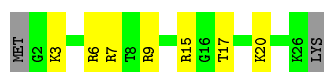
- Molecule 20: 30S ribosomal protein S20

Chain XT: 72% 22% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 67% 26% 7%



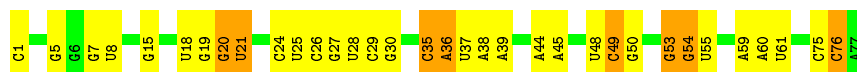
- Molecule 21: 30S ribosomal protein Thx

Chain XU: 52% 41% 7%



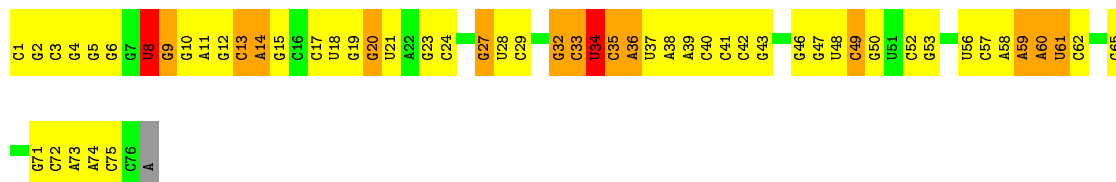
- Molecule 22: tRNA fMet

Chain QV: 56% 34% 10%



- Molecule 22: tRNA fMet

Chain QW:  26% 53% 17%



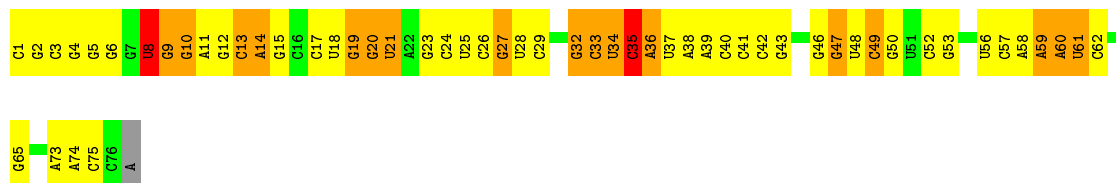
- Molecule 22: tRNA fMet

Chain XV:  58% 30% 12%



- Molecule 22: tRNA fMet

Chain XW:  26% 48% 22%



- Molecule 23: messenger RNA

Chain QX:  32% 68%



- Molecule 23: messenger RNA

Chain XX:  28% 8% 60%



- Molecule 24: ASL Leu

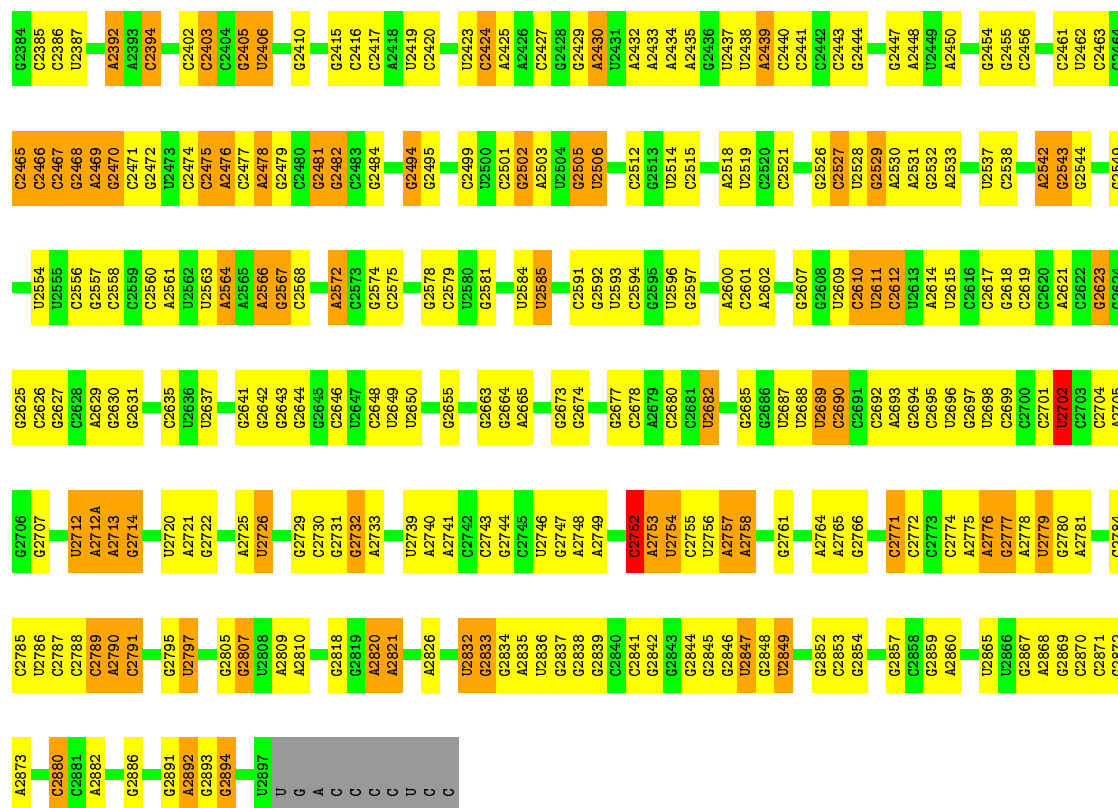
Chain QY:  59% 35% 6%



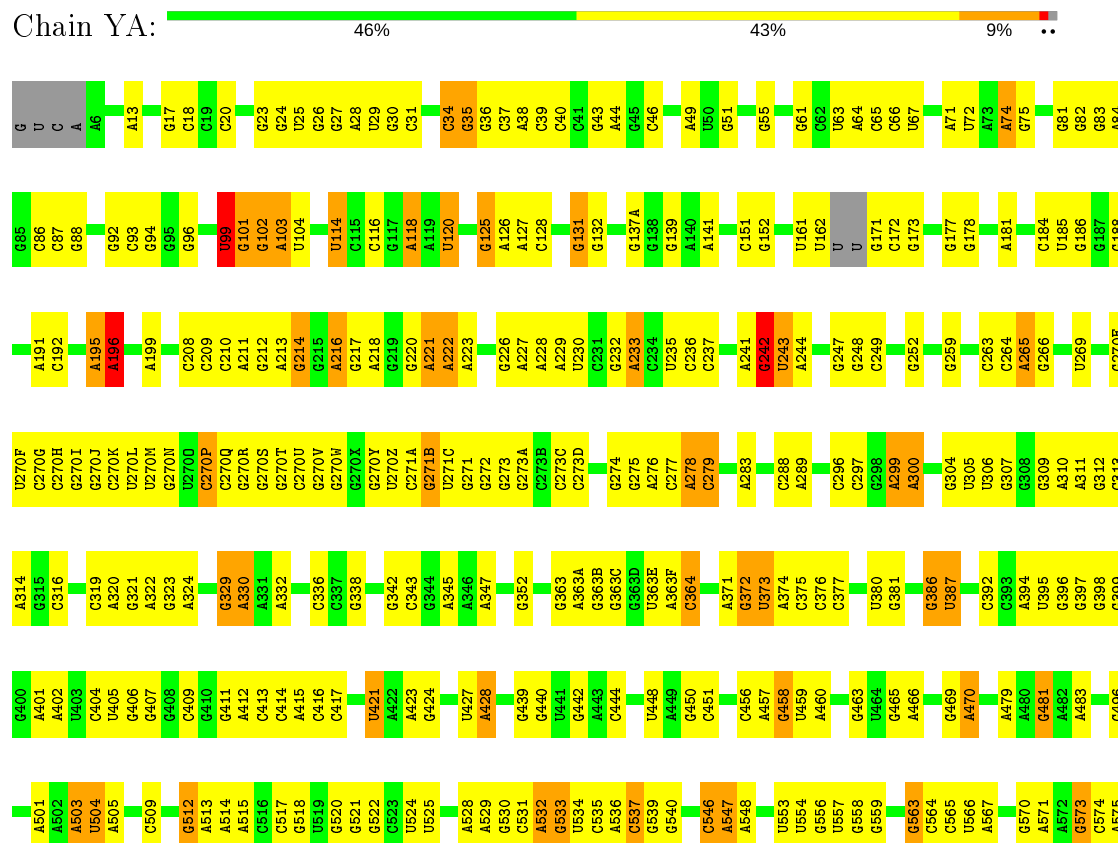
- Molecule 24: ASL Leu

Chain XY:  41% 53% 6%





- Molecule 25: 23S rRNA



| | | | | | | | | | | | | | | |
|-------|-------|--------|--------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|
| G1674 | G1591 | G1519 | A1439 | U1357 | G1264 | A1177 | U1083 | G1008 | G934 | C856 | G775 | A685 | C640 | U576 |
| C1675 | C1592 | U1520 | G1450 | G1358 | A1265 | C1178 | A1084 | A1009 | C935 | C857 | G776 | G686 | C643 | G577 |
| A1676 | G1522 | G1522 | G1441 | A1359 | G1266 | C1179 | A1085 | A1010 | G938 | U858 | | | A643 | A578 |
| A1677 | G1595 | G1525 | G1442 | A1365 | G1270 | C1180 | A1086 | A1011 | G939 | G859 | G780 | A689 | A644 | G579 |
| G1678 | A1596 | G1526 | A1444A | G1368 | G1271 | G1184 | G1087 | A1012 | G940 | U860 | A781 | G690 | C645 | C580 |
| U1680 | A1597 | G1526 | C1445 | G1380 | A1272 | G1185 | A1088 | A1013 | A941 | A661 | A782 | G691 | A646 | C581 |
| G1681 | C1598 | G1527 | C1445 | G1388 | U1273 | G1186 | G1089 | A1014 | G942 | G862 | A783 | C692 | G647 | C582 |
| G1682 | C1600 | A1528 | G1448 | U1372 | A1278 | G1187 | U1094 | G1015 | U943 | A663 | A784 | | G648 | G583 |
| C1683 | | A1529 | G1449 | A1378 | | G1191 | A1095 | G1016 | G944 | C865 | G785 | C698 | G649 | |
| C1684 | A1503 | G1530 | A1449A | A1379 | G1290 | G1192 | A1096 | G1017 | A945 | C865 | C790 | G704 | G651 | A586 |
| G1685 | C1531 | C1531 | G1453 | G1379 | C1291 | G1193 | U1097 | A1021 | G946 | A870 | C791 | | | C587 |
| G1686 | | | U1454 | G1380 | C1291 | G1194 | A1103 | G1022 | G947 | U871 | G782 | C708 | A654 | U588 |
| G1687 | G1534 | G1534 | G1455 | A1384 | U1292 | G1195 | C1104 | U1023 | G948 | A872 | G783 | U709 | G654A | C589 |
| A1688 | U1535 | U1535 | G1455 | A1385 | C1293 | C1196 | C1104 | G1024 | C949 | G873 | G784 | G710 | G | A590 |
| A1689 | C1607 | C1537 | G1458 | G1388 | G1296 | G1197 | U1108 | G1025 | G950 | G875 | G785 | G711 | G | C591 |
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| A1610 | A1510 | G1539 | A1460 | U1392 | G1298 | G1203 | G1110 | A1028 | A953 | G879 | G717 | G718 | G | G593 |
| | | G1540 | G1461 | A1392 | G1299 | A1204 | A1111 | A1029 | | G880 | | | C | U594 |
| G1613 | G1613 | U1541 | C1464 | A1393 | U1300 | U1205 | G1112 | | U958 | G881 | | | C | G598 |
| A1616 | C1617 | G1542 | C1467 | U1394 | A1301 | G1206 | U1113 | U1033 | A959 | G882 | G805 | C719 | C | G599 |
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| | | A1545A | A1471 | G1400 | G1309 | G1215 | G1116 | G1044 | C964 | G886 | C822 | U724 | C | A603 |
| G1725 | U1629 | C1547 | A1471 | G1401 | G1310 | G1216 | G1117 | G1045 | C965 | G887 | G822 | G725 | C | G604 |
| U1727 | G1636 | G1550 | G1474 | G1402 | U1313 | A1220 | G1135 | A1046 | U968 | C888 | U813 | G726 | G | G605 |
| G1728 | A1637 | G1475 | G1476 | G1403 | G1314 | | G1136 | G1047 | G969 | C889 | U807 | G727 | G | U606 |
| A1729 | C1638 | C1551 | A1477 | G1404 | C1315 | | G1137 | G1048 | U969 | C890 | G808 | A722 | C | G607 |
| U1730 | U1639 | C1557 | G1478 | U1405 | U1316 | G1226 | G1138 | G1049 | C971 | C891 | G809 | G723 | C | A602 |
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| A1641 | G1642 | G1559 | G1480 | C1407 | C1318 | G1228 | G1140 | G1055 | G973 | C893 | U813 | G729 | C | G604 |
| | | G1560 | U1482 | C1408 | G1319 | U1431 | U1141 | G1059 | C974A | A898 | C816 | G730 | C | A608 |
| G1742 | | G1561 | G1483 | C1409 | G1320 | G1230 | U1142 | U1060 | G975 | A900 | C817 | | C | A609 |
| G1743 | C1646 | A1562 | A1490 | G1410 | A1321 | G1231 | U1143 | U1061 | | | G818 | | G654S | G609A |
| A1749 | C1647 | G1563 | A1490 | C1411 | A1322 | G1232 | A142A | U1062 | G978 | G906 | U827 | A734 | | C610 |
| G1750 | G1649 | C1564 | C1493 | A1412 | | G1236 | G1144 | G1063 | G979 | U907 | U828 | U747 | U657 | U614 |
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| G1753 | A1562 | G1568 | U1497 | C1417 | C1332 | G1243 | G1154 | U1066 | A984 | C914 | C834 | A752 | U667 | G620 |
| C1754 | G1653 | A1569 | C1498 | G1418 | C1333 | | A1156 | A1067 | | C915 | A835 | C753 | G668 | G623 |
| A1755 | A1654 | C1499 | A1419 | G1420 | G1334 | A1246 | A1156 | G1068 | G993 | G916 | C754 | C754 | G669 | G624 |
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| G1758 | C1657 | A1578 | G1423 | G1424 | G1344 | C1251 | G1171 | A1071 | | | | G760 | C672 | G628 |
| C1658 | U1659 | A1579 | A1506 | G1425 | C1345 | G1252 | U1165 | C1072 | G997 | U922 | G845 | A761 | C673 | G629 |
| A1762 | C1660 | A1580 | A1507 | G1426 | C1346 | A1253 | C1166 | A1073 | C998 | C923 | C846 | A764 | G674 | G630 |
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| G1764 | C1662 | | A1510 | A1427 | G1348 | U1255 | G1168 | C1075 | A1001 | C925 | G848 | A676 | | A632 |
| C1663 | G1663 | G1585 | A1511 | C1428 | A1349 | G1257 | G1169 | G1076 | G1002 | G929 | A849 | C766 | C679 | G633 |
| | | A1586 | G1512 | G1429 | A1349 | C1257 | G1171 | A1077 | G1003 | U930 | C850 | U767 | G680 | C634 |
| U1766 | A1668 | A1587 | C1513 | C1430 | U1352 | C1258 | G1173 | U1078 | C1004 | U931 | U851 | C768 | G681 | C635 |
| C1767 | A1669 | C1588 | U1514 | U1431 | A1354 | | A1174 | C1079 | C1005 | G931 | U852 | | G682 | G636 |
| | G1770 | C1589 | C1514 | U1431 | A1354 | U1262 | U1175 | U1080 | C1006 | G932 | G853 | U773 | C683 | A637 |
| G1771 | | U1590 | C1518 | U1438 | | U1263 | G1176 | U1082 | C1007 | A933 | | A774 | G684 | U639 |

| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2892 | G2794 | G2635 | G2540 | G2454 | A2361 | C2283 | G2182 | C2107 | G2038 | A1960 | G1858 | G1772 |
| G2893 | G2795 | C2638 | A2541 | G2455 | G2362 | A2287 | C2183 | C2108 | C2039 | A1963 | A1859 | A1773 |
| G2894 | G2796 | G2638 | A2542 | C2456 | C2363 | A2288 | C2184 | U2109 | U2040 | U1964 | G1860 | U1779 |
| U2897 | G2797 | G2638 | G2543 | G2457 | G2364 | G2289 | C2185 | G2110 | G2041 | G1965 | A1780 | C1781 |
| U | A2799 | G2641 | G2544 | U2462 | G2365 | G2290 | G2186 | G2111 | C2042 | A1966 | G1862 | C1782 |
| G | C2803 | G2642 | G2545 | C2463 | A2369 | G2291 | G2187 | G2112 | G2043 | C1967 | G1863 | C1783 |
| C | C2804 | C2646 | U2546 | A2469 | U2370 | U2291 | G2190 | U2113 | G2044 | G1968 | U1864 | A1784 |
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| C | G2806 | C2648 | G2548 | C2471 | G2380 | C2293 | G2192 | G2115 | G2048 | A1970 | C1870 | A1786 |
| C | U2808 | U2649 | G2549 | G2472 | G2383 | C2294 | G2193 | G2116 | G2049 | A1971 | A1871 | A1787 |
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| U | A2810 | C2474 | U2555 | C2475 | C2385 | A2298 | G2194 | U2118 | A2051 | G1980 | G1878 | A1789 |
| C | A2740 | C2475 | C2558 | C2476 | A2392 | G2303 | A2199 | U2119 | G2052 | A1981 | C1879 | C1790 |
| C | A2741 | A2476 | C2558 | A2477 | A2393 | G2304 | A2199 | G2120 | C2055 | A1982 | C1882 | A1791 |
| C | C2742 | C2477 | U2563 | C2478 | C2394 | A2305 | U2208 | G2123 | C2056 | G1992 | C1883 | G1792 |
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| C | G2744 | A2564 | U2564 | G2482 | C2402 | G2307 | G2210 | G2125 | A2059 | G1994 | A1884 | U1794 |
| C | C2745 | A2565 | A2565 | G2482 | C2403 | G2308 | G2211 | A2126 | A2060 | C1995 | G1888 | C1795 |
| C | U2746 | A2566 | A2566 | U2492 | U2406 | G2309 | G2212 | A2127 | A2061 | U1996 | G1889 | U1796 |
| C | A2748 | C2567 | C2568 | U2493 | U2407 | A2310 | G2213 | G2128 | A2062 | G1997 | A1889 | U1797 |
| C | A2749 | C2568 | C2568 | G2494 | U2408 | A2311 | G2215 | G2129 | A2063 | U1998 | G1890 | U1798 |
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| C | C2752 | G2578 | C2578 | G2503 | G2416 | G2315 | G2231 | U2133 | G2067 | G2000 | A1903 | A1803 |
| C | A2753 | A2679 | C2575 | U2503 | C2417 | C2316 | U2232 | G2134 | A2068 | A2001 | G1906 | C1804 |
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| C | C2755 | G2681 | A2577 | G2505 | C2417 | C2318 | G2234 | G2136 | G2070 | G2003 | G1908 | A1812 |
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| C | C2757 | C2683 | C2578 | C2507 | G2418 | A2320 | G2236 | C2143 | G2072 | C2008 | C1914 | G1817 |
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| C | U2762 | U2688 | C2594 | C2515 | A2426 | G2329 | G2241 | G2152 | G2079 | G2014 | G1922 | A1825 |
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| C | A2764 | C2692 | A2602 | C2517 | G2428 | G2331 | U2243 | G2154 | C2081 | G2016 | G1935 | C1832 |
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| C | G2766 | G2694 | U2604 | U2519 | A2430 | A2335 | U2245 | G2156 | G2094 | A2019 | U1939 | G1835 |
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| C | A2774 | U2696 | A2434 | C2521 | A2435 | G2340 | A2247 | G2158 | G2087 | C2021 | G1930 | G1842 |
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| C | A2778 | G2700 | G2525 | G2525 | U2439 | G2344 | A2266 | G2164 | U2092 | C2025 | A1936 | G1846 |
| C | U2779 | C2701 | G2526 | G2526 | U2440 | A2345 | A2267 | G2165 | G2093 | C2026 | U1939 | A1847 |
| C | G2780 | U2702 | C2527 | C2527 | C2441 | A2346 | A2271 | G2166 | G2094 | G2027 | U1939 | A1848 |
| C | A2781 | A2705 | U2528 | U2528 | C2442 | C2347 | G2272 | U2167 | G2094 | U2028 | U1946 | G1958 |
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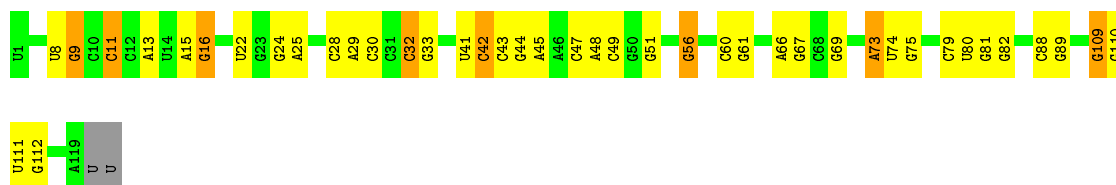
• Molecule 26: 5S rRNA

Chain RB:

64%

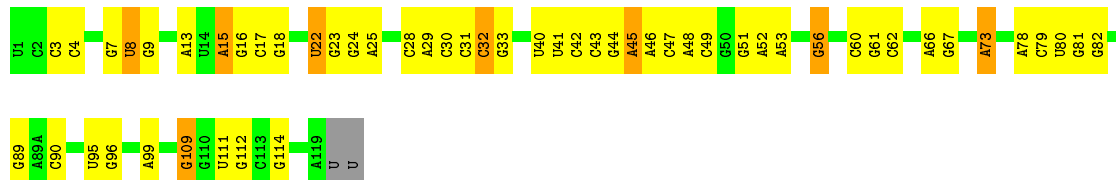
28%

7%



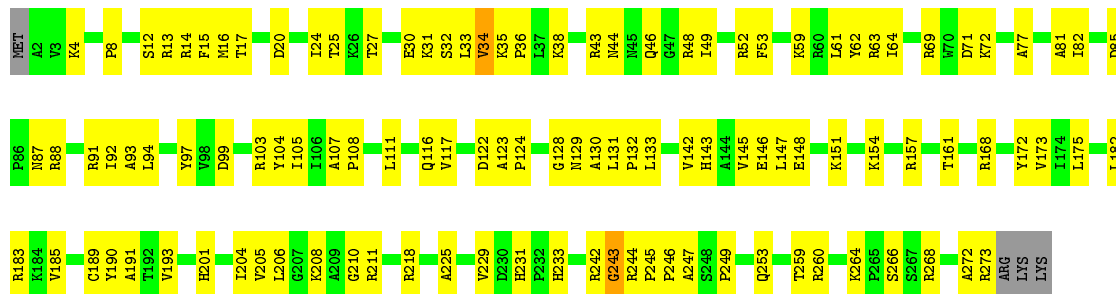
• Molecule 26: 5S rRNA

Chain YB: 54% 38% 7% .



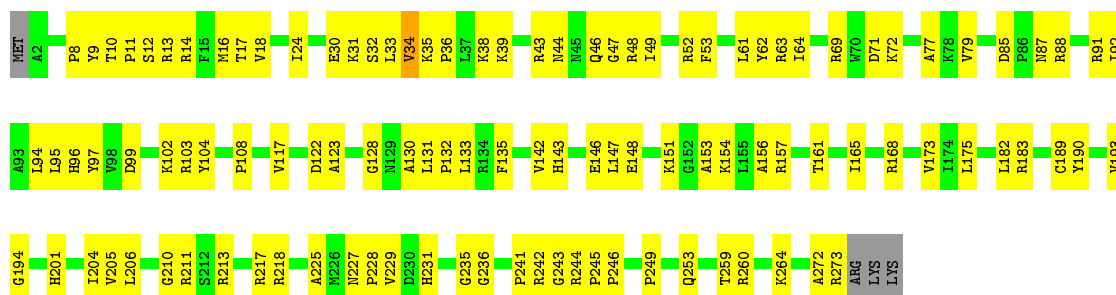
• Molecule 27: 50S ribosomal protein L2

Chain RD: 58% 40% ..



• Molecule 27: 50S ribosomal protein L2

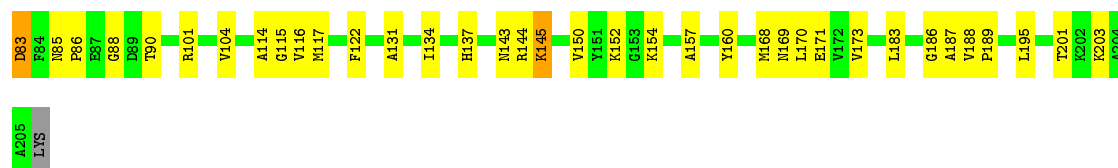
Chain YD: 59% 39% .



• Molecule 28: 50S ribosomal protein L3

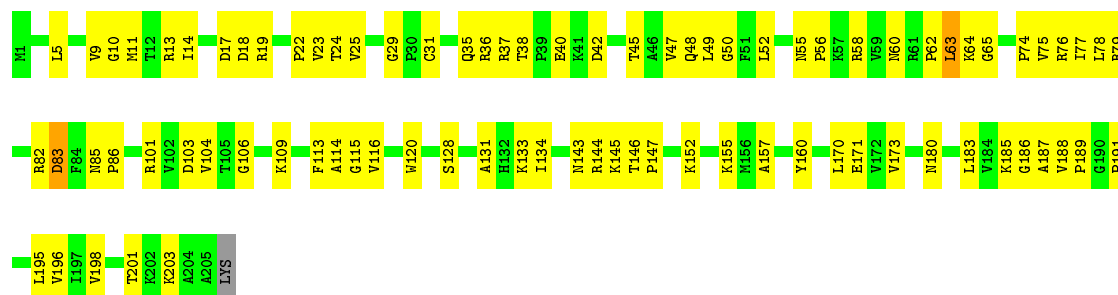
Chain RE: 61% 37% .





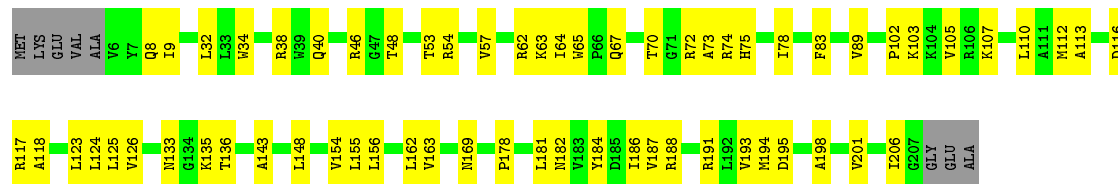
- Molecule 28: 50S ribosomal protein L3

Chain YE: 59% 40%



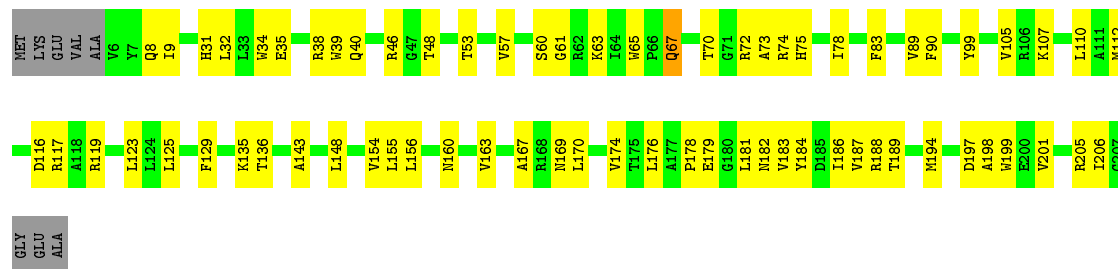
- Molecule 29: 50S ribosomal protein L4

Chain RF: 66% 30%



- Molecule 29: 50S ribosomal protein L4

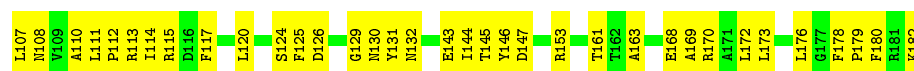
Chain YF: 63% 32%



- Molecule 30: 50S ribosomal protein L5

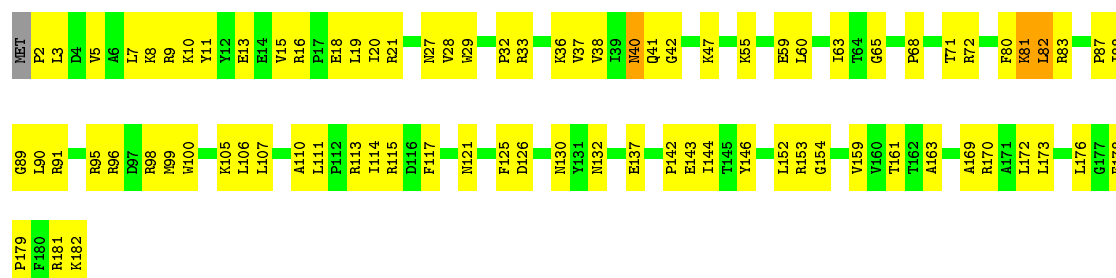
Chain RG: 59% 40%





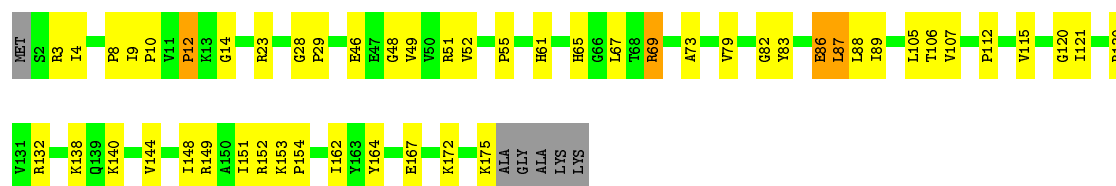
- Molecule 30: 50S ribosomal protein L5

Chain YG: 54% 44% ..



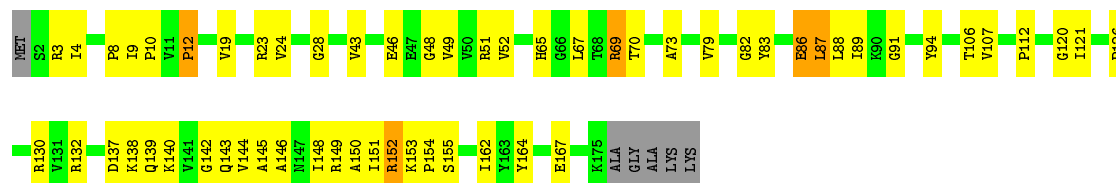
- Molecule 31: 50S ribosomal protein L6

Chain RH: 68% 26% ..



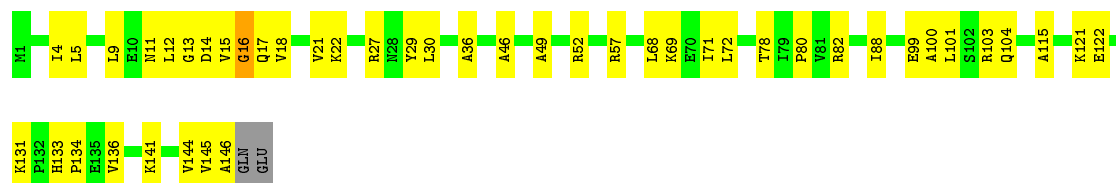
- Molecule 31: 50S ribosomal protein L6

Chain YH: 64% 29% ..



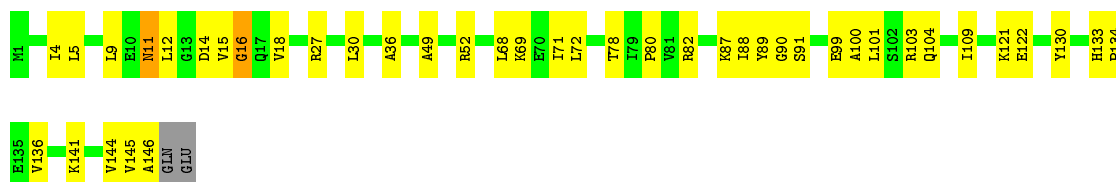
- Molecule 32: 50S ribosomal protein L9

Chain RI: 68% 30% ..



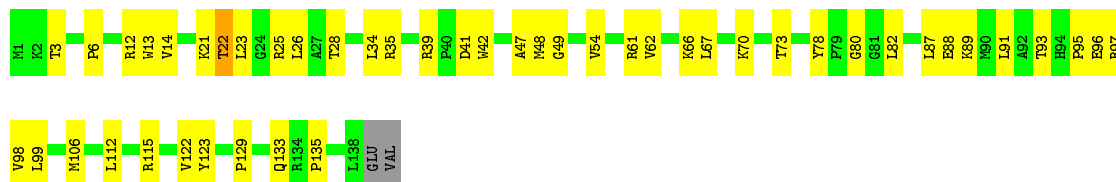
- Molecule 32: 50S ribosomal protein L9

Chain YI: 70% 27% ..



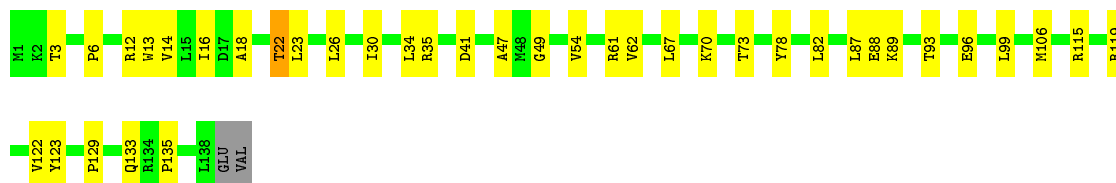
- Molecule 33: 50S ribosomal protein L13

Chain RN: 65% 33% ..



- Molecule 33: 50S ribosomal protein L13

Chain YN: 71% 26% ..



- Molecule 34: 50S ribosomal protein L14

Chain RO: 71% 28% .



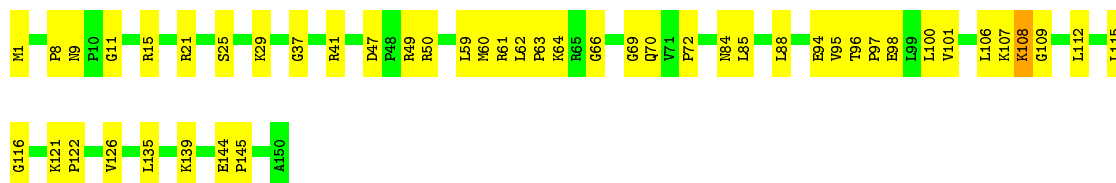
- Molecule 34: 50S ribosomal protein L14

Chain YO: 78% 21% .



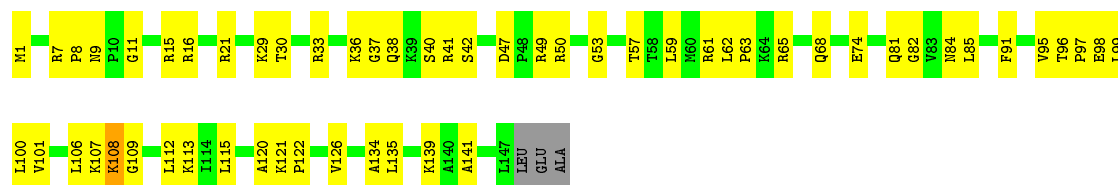
- Molecule 35: 50S ribosomal protein L15

Chain RP: 69% 31% .



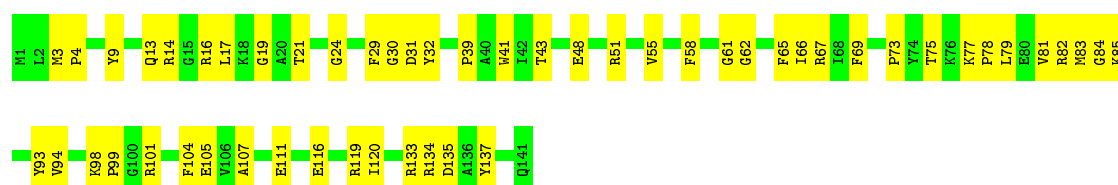
- Molecule 35: 50S ribosomal protein L15

Chain YP:  61% 37% ..



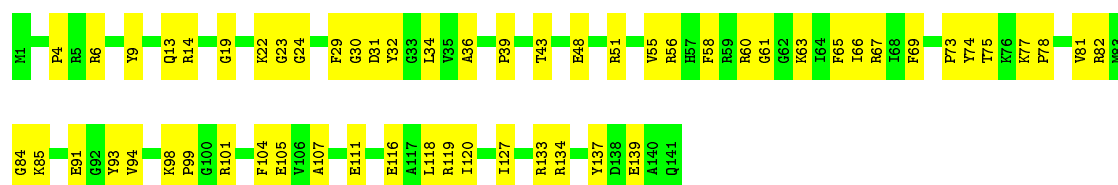
- Molecule 36: 50S ribosomal protein L16

Chain RQ:  62% 38%



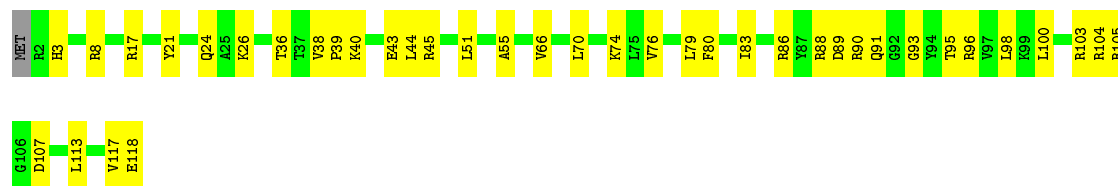
- Molecule 36: 50S ribosomal protein L16

Chain YQ:  60% 40%



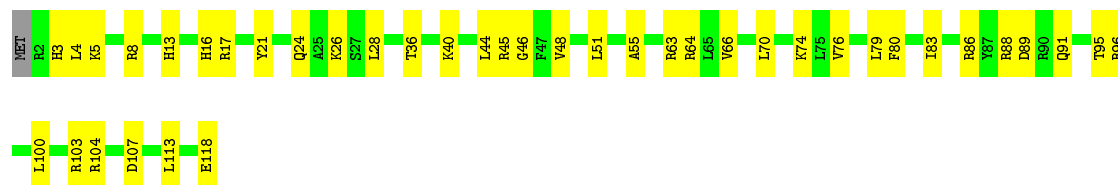
- Molecule 37: 50S ribosomal protein L17

Chain RR:  66% 33% .



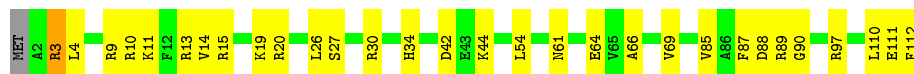
- Molecule 37: 50S ribosomal protein L17

Chain YR:  65% 34% .



- Molecule 38: 50S ribosomal protein L18

Chain RS:  72% 26% ..



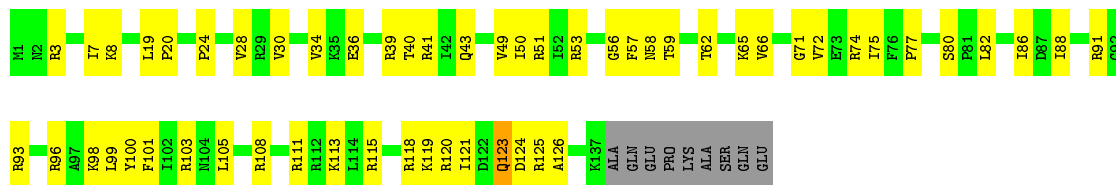
- Molecule 38: 50S ribosomal protein L18

Chain YS:  71% 28% ..



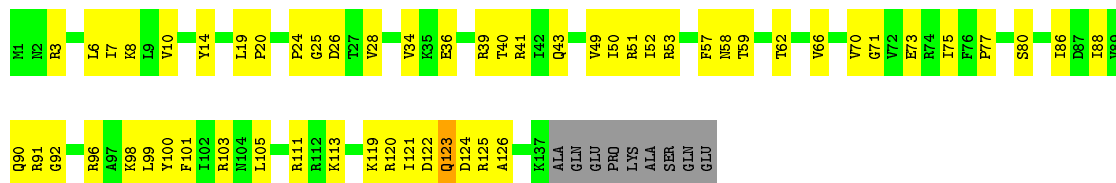
- Molecule 39: 50S ribosomal protein L19

Chain RT:  56% 37% 6%



- Molecule 39: 50S ribosomal protein L19

Chain YT:  55% 38% 6%



- Molecule 40: 50S ribosomal protein L20

Chain RU:  70% 27% ..

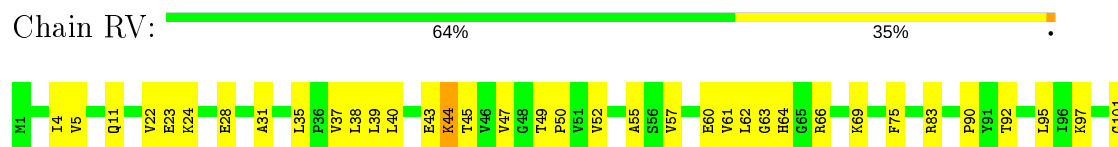


- Molecule 40: 50S ribosomal protein L20

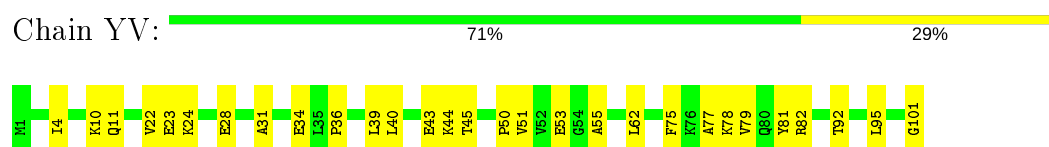
Chain YU:  70% 27% ..



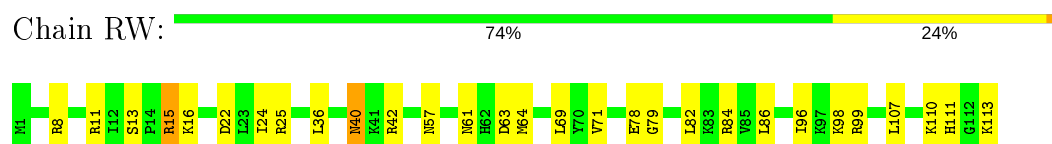
- Molecule 41: 50S ribosomal protein L21



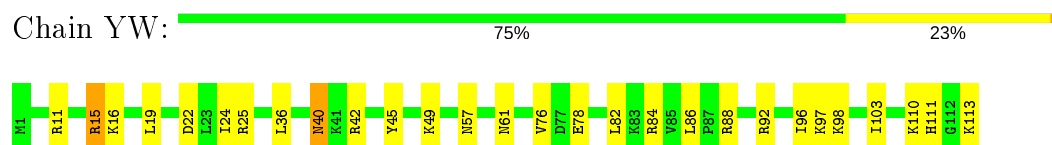
- Molecule 41: 50S ribosomal protein L21



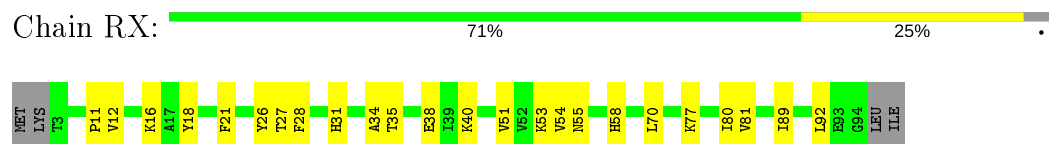
- Molecule 42: 50S ribosomal protein L22



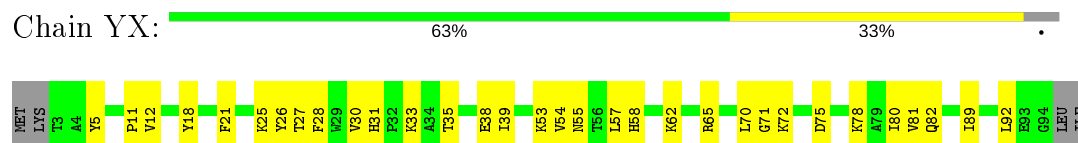
- Molecule 42: 50S ribosomal protein L22



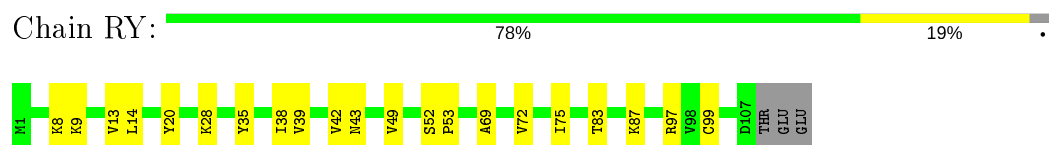
- Molecule 43: 50S ribosomal protein L23




- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24



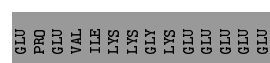
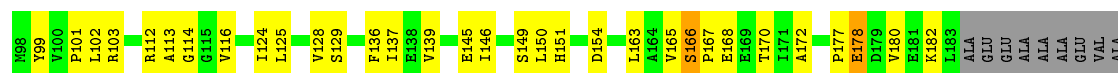
- Molecule 44: 50S ribosomal protein L24

Chain YY:  76% 21% .



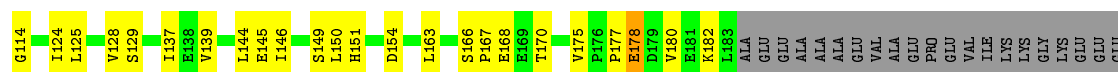
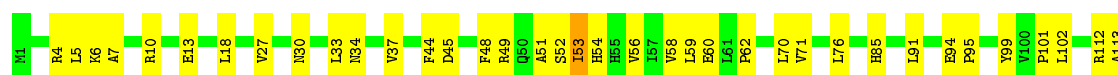
- Molecule 45: 50S ribosomal protein L25

Chain RZ:  56% 32% . 11%



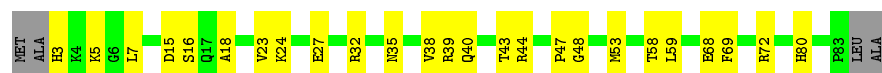
- Molecule 45: 50S ribosomal protein L25

Chain YZ:  59% 29% . 11%



- Molecule 46: 50S ribosomal protein L27

Chain R0:  66% 29% 5%



- Molecule 46: 50S ribosomal protein L27

Chain Y0:  59% 28% . 12%



- Molecule 47: 50S ribosomal protein L28

Chain R1:  73% 26% .



- Molecule 47: 50S ribosomal protein L28

Chain Y1: 61% 34% 5%



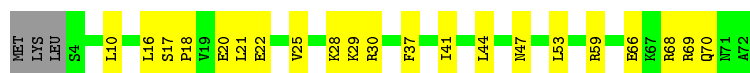
- Molecule 48: 50S ribosomal protein L29

Chain R2: 71% 25% 4%



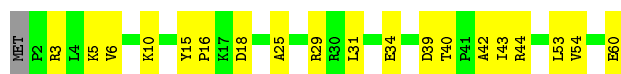
- Molecule 48: 50S ribosomal protein L29

Chain Y2: 67% 29% 4%



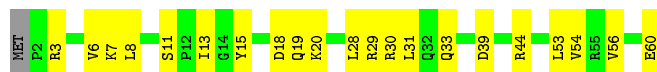
- Molecule 49: 50S ribosomal protein L30

Chain R3: 67% 32% 1%



- Molecule 49: 50S ribosomal protein L30

Chain Y3: 63% 35% 2%



- Molecule 50: 50S ribosomal protein L31

Chain R4: 69% 25% 6%



- Molecule 50: 50S ribosomal protein L31

Chain Y4: 66% 27% 7%



- Molecule 51: 50S ribosomal protein L32

Chain R5: 90% 8% .



- Molecule 51: 50S ribosomal protein L32

Chain Y5: 85% 13% .



- Molecule 52: 50S ribosomal protein L33

Chain R6: 81% 17% .



- Molecule 52: 50S ribosomal protein L33

Chain Y6: 89% 9% .



- Molecule 53: 50S ribosomal protein L34

Chain R7: 63% 33% .



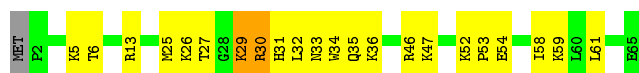
- Molecule 53: 50S ribosomal protein L34

Chain Y7: 71% 27% .

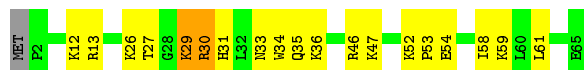


- Molecule 54: 50S ribosomal protein L35

Chain R8: 65% 31% . .



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



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 | 210.70Å 446.14Å 616.00Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 145.57 – 3.68 | Depositor |
| % Data completeness (in resolution range) | 99.3 (145.57-3.68) | Depositor |
| R_{merge} | 0.30 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.29 (at 3.58Å) | Xtriage |
| Refinement program | PHENIX 1.12_2829 | Depositor |
| R, R_{free} | 0.228 , 0.274 | Depositor |
| Wilson B-factor (Å ²) | 89.7 | Xtriage |
| Anisotropy | 0.196 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 295575 | wwPDB-VP |
| Average B, all atoms (Å ²) | 106.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, ZN, SF4

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 | QA | 0.22 | 0/36097 | 0.80 | 21/56339 (0.0%) |
| 1 | XA | 0.22 | 0/36100 | 0.82 | 27/56344 (0.0%) |
| 2 | QB | 0.26 | 0/1942 | 0.50 | 0/2619 |
| 2 | XB | 0.25 | 0/1950 | 0.49 | 0/2630 |
| 3 | QC | 0.25 | 0/1629 | 0.47 | 0/2195 |
| 3 | XC | 0.24 | 0/1629 | 0.46 | 0/2195 |
| 4 | QD | 0.35 | 1/1733 (0.1%) | 0.49 | 1/2318 (0.0%) |
| 4 | XD | 0.26 | 0/1733 | 0.47 | 0/2318 |
| 5 | QE | 0.24 | 0/1171 | 0.48 | 0/1576 |
| 5 | XE | 0.25 | 0/1171 | 0.49 | 0/1576 |
| 6 | QF | 0.24 | 0/856 | 0.49 | 0/1154 |
| 6 | XF | 0.24 | 0/856 | 0.48 | 0/1154 |
| 7 | QG | 0.24 | 0/1276 | 0.43 | 0/1709 |
| 7 | XG | 0.24 | 0/1276 | 0.42 | 0/1709 |
| 8 | QH | 0.24 | 0/1128 | 0.45 | 0/1517 |
| 8 | XH | 0.24 | 0/1128 | 0.46 | 0/1517 |
| 9 | QI | 0.26 | 0/1029 | 0.50 | 0/1379 |
| 9 | XI | 0.27 | 0/1017 | 0.52 | 0/1365 |
| 10 | QJ | 0.45 | 1/814 (0.1%) | 0.63 | 3/1095 (0.3%) |
| 10 | XJ | 0.24 | 0/790 | 0.49 | 0/1063 |
| 11 | QK | 0.25 | 0/900 | 0.46 | 0/1213 |
| 11 | XK | 0.24 | 0/879 | 0.47 | 0/1187 |
| 12 | QL | 0.26 | 0/991 | 0.59 | 0/1327 |
| 12 | XL | 0.26 | 0/972 | 0.63 | 1/1301 (0.1%) |
| 13 | QM | 0.25 | 0/965 | 0.53 | 0/1292 |
| 13 | XM | 0.24 | 0/956 | 0.53 | 0/1281 |
| 14 | QN | 0.26 | 0/501 | 0.46 | 0/664 |
| 14 | XN | 0.25 | 0/501 | 0.46 | 0/664 |
| 15 | QO | 0.24 | 0/745 | 0.43 | 0/992 |
| 15 | XO | 0.23 | 0/740 | 0.40 | 0/987 |
| 16 | QP | 0.24 | 0/721 | 0.49 | 0/970 |
| 16 | XP | 0.24 | 0/721 | 0.49 | 0/970 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | QQ | 0.24 | 0/847 | 0.46 | 0/1131 |
| 17 | XQ | 0.24 | 0/847 | 0.45 | 0/1131 |
| 18 | QR | 0.24 | 0/579 | 0.48 | 0/768 |
| 18 | XR | 0.24 | 0/579 | 0.49 | 0/768 |
| 19 | QS | 0.25 | 0/680 | 0.57 | 0/915 |
| 19 | XS | 0.26 | 0/689 | 0.57 | 0/926 |
| 20 | QT | 0.25 | 0/765 | 0.52 | 0/1007 |
| 20 | XT | 0.25 | 0/765 | 0.50 | 0/1007 |
| 21 | QU | 0.22 | 0/221 | 0.45 | 0/288 |
| 21 | XU | 0.23 | 0/221 | 0.46 | 0/288 |
| 22 | QV | 0.33 | 1/1836 (0.1%) | 0.83 | 0/2859 |
| 22 | QW | 0.26 | 0/1807 | 0.92 | 2/2816 (0.1%) |
| 22 | XV | 0.33 | 1/1836 (0.1%) | 0.84 | 1/2859 (0.0%) |
| 22 | XW | 0.26 | 0/1807 | 0.91 | 2/2816 (0.1%) |
| 23 | QX | 0.19 | 0/188 | 0.73 | 0/290 |
| 23 | XX | 0.19 | 0/235 | 0.73 | 0/364 |
| 24 | QY | 0.19 | 0/400 | 0.80 | 0/621 |
| 24 | XY | 0.20 | 0/400 | 0.79 | 0/621 |
| 25 | RA | 0.24 | 0/69521 | 0.83 | 34/108529 (0.0%) |
| 25 | YA | 0.27 | 6/69543 (0.0%) | 0.85 | 91/108563 (0.1%) |
| 26 | RB | 0.22 | 0/2878 | 0.81 | 1/4490 (0.0%) |
| 26 | YB | 0.23 | 0/2878 | 0.82 | 0/4490 |
| 27 | RD | 0.28 | 0/2165 | 0.56 | 0/2919 |
| 27 | YD | 0.28 | 0/2165 | 0.56 | 0/2919 |
| 28 | RE | 0.26 | 0/1601 | 0.60 | 1/2160 (0.0%) |
| 28 | YE | 0.26 | 0/1601 | 0.60 | 0/2160 |
| 29 | RF | 0.26 | 0/1620 | 0.50 | 0/2194 |
| 29 | YF | 0.27 | 0/1620 | 0.51 | 0/2194 |
| 30 | RG | 0.26 | 0/1499 | 0.55 | 0/2016 |
| 30 | YG | 0.26 | 0/1499 | 0.54 | 0/2016 |
| 31 | RH | 0.26 | 0/1362 | 0.57 | 1/1841 (0.1%) |
| 31 | YH | 0.29 | 0/1362 | 0.62 | 1/1841 (0.1%) |
| 32 | RI | 0.25 | 0/1151 | 0.56 | 0/1558 |
| 32 | YI | 0.25 | 0/1151 | 0.56 | 0/1558 |
| 33 | RN | 0.26 | 0/1131 | 0.58 | 0/1525 |
| 33 | YN | 0.26 | 0/1131 | 0.56 | 0/1525 |
| 34 | RO | 0.26 | 0/943 | 0.48 | 0/1269 |
| 34 | YO | 0.26 | 0/943 | 0.50 | 0/1269 |
| 35 | RP | 0.27 | 0/1162 | 0.61 | 0/1544 |
| 35 | YP | 0.27 | 0/1139 | 0.62 | 0/1514 |
| 36 | RQ | 0.26 | 0/1143 | 0.55 | 0/1527 |
| 36 | YQ | 0.26 | 0/1143 | 0.57 | 0/1527 |
| 37 | RR | 0.26 | 0/974 | 0.52 | 0/1302 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | YR | 0.25 | 0/974 | 0.49 | 0/1302 |
| 38 | RS | 0.25 | 0/892 | 0.54 | 0/1187 |
| 38 | YS | 0.25 | 0/892 | 0.54 | 0/1187 |
| 39 | RT | 0.25 | 0/1155 | 0.53 | 0/1542 |
| 39 | YT | 0.25 | 0/1155 | 0.54 | 0/1542 |
| 40 | RU | 0.26 | 0/982 | 0.51 | 0/1306 |
| 40 | YU | 0.26 | 0/982 | 0.51 | 0/1306 |
| 41 | RV | 0.26 | 0/790 | 0.58 | 0/1057 |
| 41 | YV | 0.26 | 0/790 | 0.58 | 0/1057 |
| 42 | RW | 0.25 | 0/911 | 0.50 | 0/1220 |
| 42 | YW | 0.25 | 0/911 | 0.50 | 0/1220 |
| 43 | RX | 0.26 | 0/739 | 0.48 | 0/993 |
| 43 | YX | 0.26 | 0/739 | 0.48 | 0/993 |
| 44 | RY | 0.26 | 0/831 | 0.48 | 0/1108 |
| 44 | YY | 0.26 | 0/831 | 0.51 | 0/1108 |
| 45 | RZ | 0.25 | 0/1493 | 0.63 | 0/2026 |
| 45 | YZ | 0.26 | 0/1493 | 0.64 | 0/2026 |
| 46 | R0 | 0.24 | 0/652 | 0.47 | 0/867 |
| 46 | Y0 | 0.25 | 0/607 | 0.48 | 0/809 |
| 47 | R1 | 0.27 | 0/770 | 0.55 | 0/1022 |
| 47 | Y1 | 0.29 | 0/736 | 0.53 | 0/978 |
| 48 | R2 | 0.24 | 0/583 | 0.49 | 0/771 |
| 48 | Y2 | 0.24 | 0/583 | 0.51 | 0/771 |
| 49 | R3 | 0.24 | 0/474 | 0.48 | 0/635 |
| 49 | Y3 | 0.25 | 0/474 | 0.48 | 0/635 |
| 50 | R4 | 0.25 | 0/578 | 0.53 | 0/776 |
| 50 | Y4 | 0.27 | 0/578 | 0.54 | 0/776 |
| 51 | R5 | 0.26 | 0/473 | 0.48 | 0/639 |
| 51 | Y5 | 0.25 | 0/473 | 0.46 | 0/639 |
| 52 | R6 | 0.22 | 0/460 | 0.47 | 0/613 |
| 52 | Y6 | 0.22 | 0/460 | 0.47 | 0/613 |
| 53 | R7 | 0.24 | 0/417 | 0.48 | 0/550 |
| 53 | Y7 | 0.24 | 0/426 | 0.49 | 0/561 |
| 54 | R8 | 0.33 | 0/525 | 0.67 | 0/691 |
| 54 | Y8 | 0.33 | 0/525 | 0.67 | 0/691 |
| 55 | R9 | 0.27 | 0/310 | 0.64 | 0/407 |
| 55 | Y9 | 0.63 | 0/310 | 1.20 | 2/407 (0.5%) |
| All | All | 0.25 | 10/319918 (0.0%) | 0.76 | 189/478576 (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 |
|-----|-------|---------------------|---------------------|
| 28 | YE | 0 | 2 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 22 | XV | 1 | C | OP3-P | -10.62 | 1.48 | 1.61 |
| 22 | QV | 1 | C | OP3-P | -10.59 | 1.48 | 1.61 |
| 10 | QJ | 84 | GLN | CD-NE2 | 9.70 | 1.57 | 1.32 |
| 4 | QD | 119 | GLN | CB-CG | 9.68 | 1.78 | 1.52 |
| 25 | YA | 2743 | C | P-O5' | 7.27 | 1.67 | 1.59 |
| 25 | YA | 2743 | C | C5'-C4' | 7.22 | 1.60 | 1.51 |
| 25 | YA | 2743 | C | C4'-C3' | 5.68 | 1.59 | 1.53 |
| 25 | YA | 2742 | C | O3'-P | 5.55 | 1.67 | 1.61 |
| 25 | YA | 2742 | C | C3'-O3' | 5.44 | 1.49 | 1.42 |
| 25 | YA | 2744 | G | N9-C4 | 5.24 | 1.42 | 1.38 |

All (189) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 25 | YA | 2743 | C | O4'-C1'-N1 | 17.82 | 122.46 | 108.20 |
| 25 | YA | 2755 | C | OP1-P-OP2 | 12.48 | 138.32 | 119.60 |
| 25 | YA | 2754 | U | OP1-P-O3' | -11.78 | 79.29 | 105.20 |
| 25 | YA | 2525 | G | O4'-C1'-N9 | 11.27 | 117.22 | 108.20 |
| 25 | YA | 2754 | U | OP2-P-O3' | -11.23 | 80.50 | 105.20 |
| 55 | Y9 | 29 | ASN | C-N-CD | -10.53 | 97.44 | 120.60 |
| 25 | YA | 2525 | G | N9-C4-C5 | 10.39 | 109.56 | 105.40 |
| 25 | YA | 2741 | A | P-O3'-C3' | 10.11 | 131.83 | 119.70 |
| 25 | YA | 2743 | C | O5'-P-OP2 | 9.69 | 122.33 | 110.70 |
| 25 | YA | 2744 | G | N3-C4-C5 | -9.02 | 124.09 | 128.60 |
| 25 | YA | 2525 | G | C6-N1-C2 | -8.68 | 119.89 | 125.10 |
| 25 | YA | 2525 | G | C2-N3-C4 | 8.63 | 116.22 | 111.90 |
| 25 | YA | 2525 | G | C4-C5-N7 | -8.33 | 107.47 | 110.80 |
| 25 | YA | 2755 | C | C5-C4-N4 | -8.12 | 114.52 | 120.20 |
| 1 | QA | 1158 | C | C2-N1-C1' | 7.85 | 127.43 | 118.80 |
| 25 | YA | 2744 | G | N3-C4-N9 | 7.77 | 130.66 | 126.00 |
| 25 | YA | 2755 | C | C5-C6-N1 | 7.76 | 124.88 | 121.00 |
| 25 | YA | 2743 | C | C6-N1-C2 | -7.67 | 117.23 | 120.30 |
| 25 | YA | 2527 | C | C2-N1-C1' | 7.58 | 127.14 | 118.80 |
| 1 | QA | 1158 | C | N1-C2-O2 | 7.48 | 123.39 | 118.90 |
| 25 | YA | 2525 | G | C8-N9-C1' | 7.47 | 136.72 | 127.00 |
| 1 | XA | 1158 | C | C2-N1-C1' | 7.44 | 126.98 | 118.80 |
| 25 | YA | 2747 | G | C4-C5-N7 | 7.35 | 113.74 | 110.80 |
| 25 | YA | 2527 | C | N1-C2-O2 | 7.25 | 123.25 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 25 | YA | 1396 | U | C2-N1-C1' | 7.21 | 126.36 | 117.70 |
| 25 | YA | 2506 | U | C2-N1-C1' | 7.14 | 126.27 | 117.70 |
| 25 | YA | 2356 | C | C2-N1-C1' | -7.12 | 110.97 | 118.80 |
| 1 | XA | 186(F) | C | N3-C2-O2 | -7.11 | 116.92 | 121.90 |
| 1 | XA | 163 | C | C6-N1-C1' | 7.07 | 129.29 | 120.80 |
| 25 | YA | 1313 | U | C2-N1-C1' | 7.05 | 126.17 | 117.70 |
| 25 | RA | 2702 | U | C2-N1-C1' | 7.05 | 126.16 | 117.70 |
| 25 | RA | 828 | U | C2-N1-C1' | 7.00 | 126.10 | 117.70 |
| 25 | YA | 2506 | U | N1-C2-O2 | 6.98 | 127.69 | 122.80 |
| 25 | YA | 2525 | G | C5-C6-N1 | 6.87 | 114.94 | 111.50 |
| 25 | YA | 2747 | G | N9-C4-C5 | -6.87 | 102.65 | 105.40 |
| 1 | XA | 159 | G | N3-C4-N9 | -6.83 | 121.90 | 126.00 |
| 1 | XA | 1301 | U | C2-N1-C1' | 6.81 | 125.87 | 117.70 |
| 25 | YA | 1396 | U | N1-C2-O2 | 6.80 | 127.56 | 122.80 |
| 25 | YA | 2356 | C | C6-N1-C1' | 6.79 | 128.94 | 120.80 |
| 25 | YA | 1535 | U | C2-N1-C1' | 6.75 | 125.80 | 117.70 |
| 25 | YA | 2525 | G | C6-C5-N7 | 6.75 | 134.45 | 130.40 |
| 25 | RA | 828 | U | N1-C2-O2 | 6.71 | 127.50 | 122.80 |
| 25 | YA | 2506 | U | N3-C2-O2 | -6.71 | 117.51 | 122.20 |
| 1 | XA | 1158 | C | N1-C2-O2 | 6.71 | 122.92 | 118.90 |
| 25 | YA | 2356 | C | C2-N3-C4 | -6.69 | 116.56 | 119.90 |
| 1 | QA | 1301 | U | N1-C2-O2 | 6.64 | 127.45 | 122.80 |
| 25 | RA | 1313 | U | C2-N1-C1' | 6.60 | 125.62 | 117.70 |
| 25 | RA | 2752 | C | N1-C2-O2 | 6.59 | 122.86 | 118.90 |
| 1 | XA | 386 | C | N3-C2-O2 | -6.59 | 117.29 | 121.90 |
| 25 | YA | 828 | U | C2-N1-C1' | 6.58 | 125.60 | 117.70 |
| 25 | YA | 2742 | C | O5'-P-OP1 | 6.52 | 118.52 | 110.70 |
| 1 | QA | 1066 | C | C2-N1-C1' | 6.47 | 125.91 | 118.80 |
| 25 | RA | 2484 | G | N1-C6-O6 | -6.46 | 116.03 | 119.90 |
| 25 | YA | 2742 | C | P-O3'-C3' | 6.43 | 127.41 | 119.70 |
| 25 | YA | 2743 | C | OP1-P-OP2 | -6.43 | 109.96 | 119.60 |
| 1 | XA | 163 | C | C2-N1-C1' | -6.39 | 111.77 | 118.80 |
| 25 | RA | 828 | U | N3-C2-O2 | -6.35 | 117.76 | 122.20 |
| 25 | RA | 2752 | C | C2-N1-C1' | 6.33 | 125.77 | 118.80 |
| 4 | QD | 119 | GLN | CB-CG-CD | -6.28 | 95.27 | 111.60 |
| 25 | YA | 1396 | U | N3-C2-O2 | -6.27 | 117.81 | 122.20 |
| 25 | RA | 2702 | U | N1-C2-O2 | 6.22 | 127.16 | 122.80 |
| 1 | XA | 747 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 25 | YA | 1535 | U | N1-C2-O2 | 6.14 | 127.10 | 122.80 |
| 1 | XA | 1301 | U | N1-C2-O2 | 6.11 | 127.08 | 122.80 |
| 25 | YA | 2742 | C | C6-N1-C2 | -6.10 | 117.86 | 120.30 |
| 25 | YA | 2744 | G | C2-N3-C4 | 6.09 | 114.95 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 25 | YA | 2741 | A | N7-C8-N9 | 6.03 | 116.81 | 113.80 |
| 25 | YA | 1407 | C | C2-N1-C1' | 5.92 | 125.31 | 118.80 |
| 1 | QA | 1301 | U | C2-N1-C1' | 5.91 | 124.79 | 117.70 |
| 1 | XA | 252 | U | C2-N1-C1' | 5.87 | 124.75 | 117.70 |
| 1 | XA | 163 | C | N3-C2-O2 | -5.87 | 117.79 | 121.90 |
| 25 | YA | 2755 | C | C4-C5-C6 | -5.86 | 114.47 | 117.40 |
| 1 | QA | 1301 | U | N3-C2-O2 | -5.85 | 118.10 | 122.20 |
| 25 | RA | 2506 | U | C2-N1-C1' | 5.83 | 124.70 | 117.70 |
| 25 | RA | 2506 | U | N1-C2-O2 | 5.83 | 126.88 | 122.80 |
| 25 | YA | 2539 | C | C6-N1-C2 | -5.81 | 117.97 | 120.30 |
| 1 | QA | 1066 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 25 | YA | 2527 | C | C6-N1-C1' | -5.81 | 113.83 | 120.80 |
| 1 | XA | 747 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 25 | YA | 2525 | G | C4-N9-C1' | -5.74 | 119.04 | 126.50 |
| 10 | QJ | 84 | GLN | CB-CA-C | -5.73 | 98.94 | 110.40 |
| 25 | YA | 2356 | C | N1-C2-N3 | 5.73 | 123.21 | 119.20 |
| 25 | YA | 2525 | G | N3-C2-N2 | -5.72 | 115.89 | 119.90 |
| 1 | QA | 1158 | C | N3-C2-O2 | -5.71 | 117.90 | 121.90 |
| 25 | RA | 1535 | U | C2-N1-C1' | 5.71 | 124.55 | 117.70 |
| 1 | XA | 961 | U | N1-C2-N3 | 5.69 | 118.31 | 114.90 |
| 25 | YA | 2741 | A | C8-N9-C4 | -5.68 | 103.53 | 105.80 |
| 25 | RA | 2484 | G | C5-C6-O6 | 5.65 | 131.99 | 128.60 |
| 25 | RA | 1462 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 25 | YA | 2743 | C | OP1-P-O3' | 5.64 | 117.61 | 105.20 |
| 1 | XA | 159 | G | C5-C6-O6 | 5.63 | 131.98 | 128.60 |
| 25 | YA | 2755 | C | N3-C4-N4 | 5.63 | 121.94 | 118.00 |
| 25 | RA | 2752 | C | N3-C2-O2 | -5.61 | 117.97 | 121.90 |
| 1 | XA | 1301 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |
| 1 | XA | 163 | C | N1-C2-N3 | 5.58 | 123.11 | 119.20 |
| 25 | YA | 99 | U | OP2-P-O3' | 5.58 | 117.47 | 105.20 |
| 25 | RA | 1124 | C | N3-C2-O2 | -5.57 | 118.00 | 121.90 |
| 1 | QA | 1158 | C | C6-N1-C1' | -5.56 | 114.13 | 120.80 |
| 1 | XA | 812 | C | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 1 | QA | 1027 | C | OP1-P-O3' | 5.54 | 117.39 | 105.20 |
| 25 | YA | 828 | U | N1-C2-O2 | 5.52 | 126.66 | 122.80 |
| 25 | YA | 1535 | U | N3-C2-O2 | -5.51 | 118.34 | 122.20 |
| 25 | RA | 2060 | A | P-O3'-C3' | 5.51 | 126.31 | 119.70 |
| 25 | YA | 2525 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 25 | YA | 1314 | C | C2-N1-C1' | 5.48 | 124.83 | 118.80 |
| 1 | XA | 1158 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 25 | RA | 1992 | G | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 25 | YA | 1914 | C | C2-N1-C1' | 5.45 | 124.79 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25 | YA | 2474 | C | C2-N1-C1' | 5.42 | 124.76 | 118.80 |
| 25 | YA | 2526 | G | C4-N9-C1' | 5.40 | 133.52 | 126.50 |
| 25 | YA | 2743 | C | P-O5'-C5' | 5.40 | 129.54 | 120.90 |
| 1 | XA | 163 | C | C5-C4-N4 | 5.39 | 123.98 | 120.20 |
| 31 | YH | 82 | GLY | N-CA-C | 5.39 | 126.58 | 113.10 |
| 25 | RA | 2506 | U | N3-C2-O2 | -5.39 | 118.43 | 122.20 |
| 25 | YA | 1180 | C | C2-N1-C1' | 5.37 | 124.71 | 118.80 |
| 25 | YA | 2742 | C | O5'-P-OP2 | -5.37 | 100.87 | 105.70 |
| 25 | YA | 2526 | G | N7-C8-N9 | 5.36 | 115.78 | 113.10 |
| 1 | XA | 378 | G | N3-C4-N9 | -5.35 | 122.79 | 126.00 |
| 1 | QA | 1322 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 1 | XA | 1158 | C | C6-N1-C2 | -5.31 | 118.17 | 120.30 |
| 1 | QA | 328 | C | P-O3'-C3' | 5.31 | 126.08 | 119.70 |
| 25 | YA | 2474 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 25 | YA | 2755 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 25 | RA | 1407 | C | C2-N1-C1' | 5.27 | 124.59 | 118.80 |
| 25 | RA | 2468 | G | O4'-C1'-N9 | 5.27 | 112.41 | 108.20 |
| 10 | QJ | 84 | GLN | CG-CD-OE1 | -5.26 | 111.08 | 121.60 |
| 25 | YA | 2889 | C | C2-N1-C1' | 5.26 | 124.58 | 118.80 |
| 25 | YA | 99 | U | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 1 | QA | 1027 | C | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 1 | XA | 528 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 25 | RA | 2702 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 25 | YA | 196 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 1 | XA | 328 | C | P-O3'-C3' | 5.24 | 125.98 | 119.70 |
| 22 | XW | 8 | U | OP1-P-O3' | 5.23 | 116.72 | 105.20 |
| 25 | YA | 537 | C | C2-N1-C1' | 5.23 | 124.55 | 118.80 |
| 25 | YA | 2538 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 10 | QJ | 84 | GLN | N-CA-CB | 5.22 | 120.00 | 110.60 |
| 25 | YA | 2681 | C | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 12 | XL | 46 | LYS | C-N-CA | -5.21 | 108.68 | 121.70 |
| 22 | XW | 35 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 28 | RE | 78 | LEU | CA-CB-CG | 5.20 | 127.25 | 115.30 |
| 25 | YA | 2527 | C | N3-C4-N4 | 5.19 | 121.63 | 118.00 |
| 55 | Y9 | 26 | ILE | N-CA-CB | 5.18 | 122.70 | 110.80 |
| 25 | RA | 1314 | C | C2-N1-C1' | 5.17 | 124.49 | 118.80 |
| 25 | RA | 404 | C | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 25 | YA | 1992 | G | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | QA | 792 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | QA | 812 | C | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 22 | XV | 66 | C | C2-N1-C1' | 5.16 | 124.47 | 118.80 |
| 22 | QW | 8 | U | OP1-P-O3' | 5.15 | 116.54 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 25 | YA | 2342 | C | C2-N1-C1' | 5.15 | 124.47 | 118.80 |
| 31 | RH | 82 | GLY | N-CA-C | 5.15 | 125.97 | 113.10 |
| 1 | XA | 931 | C | N3-C4-N4 | -5.14 | 114.40 | 118.00 |
| 25 | YA | 2525 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 25 | RA | 1411 | C | C2-N1-C1' | 5.14 | 124.45 | 118.80 |
| 25 | YA | 242 | G | P-O3'-C3' | 5.13 | 125.86 | 119.70 |
| 25 | YA | 669 | G | C4-N9-C1' | 5.13 | 133.17 | 126.50 |
| 25 | YA | 2539 | C | N1-C2-O2 | -5.12 | 115.83 | 118.90 |
| 25 | YA | 1313 | U | N1-C2-O2 | 5.12 | 126.38 | 122.80 |
| 25 | RA | 1914 | C | C2-N1-C1' | 5.11 | 124.42 | 118.80 |
| 1 | QA | 1297 | C | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 25 | YA | 2539 | C | N1-C2-N3 | 5.11 | 122.78 | 119.20 |
| 25 | YA | 2743 | C | P-O3'-C3' | 5.11 | 125.83 | 119.70 |
| 25 | YA | 828 | U | N3-C2-O2 | -5.11 | 118.63 | 122.20 |
| 1 | QA | 1322 | C | N1-C2-O2 | 5.10 | 121.96 | 118.90 |
| 25 | RA | 2752 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 25 | RA | 846 | C | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 25 | YA | 114 | U | C2-N1-C1' | 5.09 | 123.81 | 117.70 |
| 1 | QA | 913 | A | P-O3'-C3' | 5.09 | 125.80 | 119.70 |
| 25 | RA | 1882 | C | C2-N1-C1' | 5.09 | 124.39 | 118.80 |
| 25 | YA | 1313 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |
| 22 | QW | 34 | U | C2-N1-C1' | 5.07 | 123.78 | 117.70 |
| 1 | QA | 1346 | A | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 1 | XA | 1297 | C | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 25 | YA | 846 | C | P-O3'-C3' | 5.05 | 125.76 | 119.70 |
| 1 | QA | 1498 | U | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 25 | RA | 1558 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 25 | RA | 271(B) | G | P-O3'-C3' | 5.03 | 125.74 | 119.70 |
| 1 | XA | 449 | C | C2-N1-C1' | 5.03 | 124.34 | 118.80 |
| 25 | RA | 1022 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 25 | YA | 1686 | C | C2-N1-C1' | 5.03 | 124.33 | 118.80 |
| 25 | RA | 229 | A | OP2-P-O3' | 5.02 | 116.25 | 105.20 |
| 25 | YA | 271(B) | G | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 25 | YA | 2744 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 26 | RB | 11 | C | N3-C2-O2 | -5.02 | 118.39 | 121.90 |
| 25 | YA | 1026 | U | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 25 | RA | 229 | A | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 1 | QA | 992 | U | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 25 | YA | 1022 | G | P-O3'-C3' | 5.00 | 125.71 | 119.70 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 28 | YE | 146 | THR | Mainchain,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 | QA | 32246 | 0 | 16278 | 644 | 0 |
| 1 | XA | 32248 | 0 | 16279 | 617 | 0 |
| 2 | QB | 1907 | 0 | 1958 | 51 | 0 |
| 2 | XB | 1915 | 0 | 1969 | 47 | 0 |
| 3 | QC | 1605 | 0 | 1668 | 37 | 0 |
| 3 | XC | 1605 | 0 | 1668 | 33 | 0 |
| 4 | QD | 1703 | 0 | 1766 | 53 | 0 |
| 4 | XD | 1703 | 0 | 1767 | 46 | 0 |
| 5 | QE | 1155 | 0 | 1213 | 23 | 0 |
| 5 | XE | 1155 | 0 | 1213 | 18 | 0 |
| 6 | QF | 843 | 0 | 857 | 18 | 0 |
| 6 | XF | 843 | 0 | 857 | 22 | 0 |
| 7 | QG | 1257 | 0 | 1296 | 20 | 0 |
| 7 | XG | 1257 | 0 | 1296 | 18 | 0 |
| 8 | QH | 1108 | 0 | 1165 | 23 | 0 |
| 8 | XH | 1108 | 0 | 1165 | 20 | 0 |
| 9 | QI | 1010 | 0 | 1037 | 35 | 0 |
| 9 | XI | 998 | 0 | 1024 | 39 | 0 |
| 10 | QJ | 801 | 0 | 849 | 39 | 0 |
| 10 | XJ | 777 | 0 | 816 | 24 | 0 |
| 11 | QK | 885 | 0 | 904 | 33 | 0 |
| 11 | XK | 864 | 0 | 881 | 25 | 0 |
| 12 | QL | 975 | 0 | 1062 | 26 | 0 |
| 12 | XL | 956 | 0 | 1046 | 28 | 0 |
| 13 | QM | 955 | 0 | 1021 | 46 | 0 |
| 13 | XM | 946 | 0 | 1007 | 36 | 0 |
| 14 | QN | 492 | 0 | 529 | 15 | 0 |
| 14 | XN | 492 | 0 | 529 | 12 | 0 |
| 15 | QO | 734 | 0 | 771 | 13 | 0 |
| 15 | XO | 729 | 0 | 768 | 17 | 0 |
| 16 | QP | 705 | 0 | 725 | 19 | 0 |
| 16 | XP | 705 | 0 | 725 | 22 | 0 |
| 17 | QQ | 834 | 0 | 904 | 14 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17 | XQ | 834 | 0 | 904 | 21 | 0 |
| 18 | QR | 574 | 0 | 644 | 19 | 0 |
| 18 | XR | 574 | 0 | 644 | 22 | 0 |
| 19 | QS | 665 | 0 | 686 | 26 | 0 |
| 19 | XS | 674 | 0 | 699 | 21 | 0 |
| 20 | QT | 763 | 0 | 861 | 17 | 0 |
| 20 | XT | 763 | 0 | 861 | 19 | 0 |
| 21 | QU | 217 | 0 | 234 | 6 | 0 |
| 21 | XU | 217 | 0 | 234 | 10 | 0 |
| 22 | QV | 1644 | 0 | 836 | 21 | 0 |
| 22 | QW | 1618 | 0 | 826 | 45 | 0 |
| 22 | XV | 1644 | 0 | 836 | 19 | 0 |
| 22 | XW | 1618 | 0 | 826 | 44 | 0 |
| 23 | QX | 169 | 0 | 86 | 0 | 0 |
| 23 | XX | 210 | 0 | 109 | 3 | 0 |
| 24 | QY | 358 | 0 | 183 | 3 | 0 |
| 24 | XY | 358 | 0 | 184 | 5 | 0 |
| 25 | RA | 62071 | 0 | 31291 | 1006 | 0 |
| 25 | YA | 62091 | 0 | 31297 | 1166 | 0 |
| 26 | RB | 2573 | 0 | 1306 | 29 | 0 |
| 26 | YB | 2573 | 0 | 1306 | 42 | 0 |
| 27 | RD | 2115 | 0 | 2195 | 101 | 0 |
| 27 | YD | 2115 | 0 | 2195 | 102 | 0 |
| 28 | RE | 1568 | 0 | 1634 | 67 | 0 |
| 28 | YE | 1568 | 0 | 1634 | 64 | 0 |
| 29 | RF | 1585 | 0 | 1632 | 53 | 0 |
| 29 | YF | 1585 | 0 | 1632 | 55 | 0 |
| 30 | RG | 1474 | 0 | 1535 | 58 | 0 |
| 30 | YG | 1474 | 0 | 1535 | 69 | 0 |
| 31 | RH | 1336 | 0 | 1418 | 37 | 0 |
| 31 | YH | 1336 | 0 | 1418 | 72 | 0 |
| 32 | RI | 1136 | 0 | 1223 | 28 | 0 |
| 32 | YI | 1136 | 0 | 1223 | 27 | 0 |
| 33 | RN | 1104 | 0 | 1180 | 30 | 0 |
| 33 | YN | 1104 | 0 | 1180 | 25 | 0 |
| 34 | RO | 933 | 0 | 996 | 32 | 0 |
| 34 | YO | 933 | 0 | 996 | 26 | 0 |
| 35 | RP | 1145 | 0 | 1228 | 48 | 0 |
| 35 | YP | 1122 | 0 | 1206 | 50 | 0 |
| 36 | RQ | 1122 | 0 | 1179 | 49 | 0 |
| 36 | YQ | 1122 | 0 | 1179 | 47 | 0 |
| 37 | RR | 960 | 0 | 1021 | 30 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37 | YR | 960 | 0 | 1021 | 27 | 0 |
| 38 | RS | 882 | 0 | 943 | 23 | 0 |
| 38 | YS | 882 | 0 | 943 | 27 | 0 |
| 39 | RT | 1141 | 0 | 1202 | 46 | 0 |
| 39 | YT | 1141 | 0 | 1202 | 49 | 0 |
| 40 | RU | 964 | 0 | 1022 | 47 | 0 |
| 40 | YU | 964 | 0 | 1022 | 45 | 0 |
| 41 | RV | 779 | 0 | 852 | 31 | 0 |
| 41 | YV | 779 | 0 | 852 | 24 | 0 |
| 42 | RW | 900 | 0 | 964 | 21 | 1 |
| 42 | YW | 900 | 0 | 964 | 21 | 0 |
| 43 | RX | 725 | 0 | 778 | 17 | 0 |
| 43 | YX | 725 | 0 | 778 | 25 | 0 |
| 44 | RY | 818 | 0 | 910 | 13 | 0 |
| 44 | YY | 818 | 0 | 912 | 14 | 1 |
| 45 | RZ | 1461 | 0 | 1493 | 46 | 0 |
| 45 | YZ | 1461 | 0 | 1493 | 46 | 0 |
| 46 | R0 | 643 | 0 | 667 | 20 | 0 |
| 46 | Y0 | 599 | 0 | 617 | 23 | 0 |
| 47 | R1 | 763 | 0 | 848 | 18 | 0 |
| 47 | Y1 | 729 | 0 | 802 | 22 | 0 |
| 48 | R2 | 581 | 0 | 629 | 12 | 0 |
| 48 | Y2 | 581 | 0 | 629 | 14 | 0 |
| 49 | R3 | 469 | 0 | 518 | 14 | 0 |
| 49 | Y3 | 469 | 0 | 518 | 16 | 0 |
| 50 | R4 | 565 | 0 | 557 | 18 | 0 |
| 50 | Y4 | 565 | 0 | 558 | 25 | 0 |
| 51 | R5 | 459 | 0 | 477 | 5 | 0 |
| 51 | Y5 | 459 | 0 | 480 | 10 | 0 |
| 52 | R6 | 453 | 0 | 474 | 7 | 0 |
| 52 | Y6 | 453 | 0 | 473 | 3 | 0 |
| 53 | R7 | 409 | 0 | 454 | 12 | 0 |
| 53 | Y7 | 418 | 0 | 467 | 9 | 0 |
| 54 | R8 | 517 | 0 | 582 | 22 | 0 |
| 54 | Y8 | 517 | 0 | 582 | 21 | 0 |
| 55 | R9 | 307 | 0 | 338 | 22 | 0 |
| 55 | Y9 | 307 | 0 | 338 | 141 | 0 |
| 56 | QA | 68 | 0 | 0 | 0 | 0 |
| 56 | QC | 1 | 0 | 0 | 0 | 0 |
| 56 | QE | 1 | 0 | 0 | 0 | 0 |
| 56 | QF | 1 | 0 | 0 | 0 | 0 |
| 56 | QH | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | QQ | 1 | 0 | 0 | 0 | 0 |
| 56 | QV | 6 | 0 | 0 | 0 | 0 |
| 56 | QY | 1 | 0 | 0 | 0 | 0 |
| 56 | R0 | 4 | 0 | 0 | 0 | 0 |
| 56 | R1 | 2 | 0 | 0 | 0 | 0 |
| 56 | R4 | 1 | 0 | 0 | 0 | 0 |
| 56 | R8 | 1 | 0 | 0 | 0 | 0 |
| 56 | R9 | 1 | 0 | 0 | 0 | 0 |
| 56 | RA | 508 | 0 | 0 | 0 | 0 |
| 56 | RB | 7 | 0 | 0 | 0 | 0 |
| 56 | RE | 2 | 0 | 0 | 0 | 0 |
| 56 | RF | 1 | 0 | 0 | 0 | 0 |
| 56 | RN | 1 | 0 | 0 | 0 | 0 |
| 56 | RO | 2 | 0 | 0 | 0 | 0 |
| 56 | RP | 2 | 0 | 0 | 0 | 0 |
| 56 | RQ | 2 | 0 | 0 | 0 | 0 |
| 56 | RR | 1 | 0 | 0 | 0 | 0 |
| 56 | RT | 1 | 0 | 0 | 0 | 0 |
| 56 | RU | 1 | 0 | 0 | 0 | 0 |
| 56 | RY | 1 | 0 | 0 | 0 | 0 |
| 56 | XA | 82 | 0 | 0 | 0 | 0 |
| 56 | XE | 1 | 0 | 0 | 0 | 0 |
| 56 | XL | 1 | 0 | 0 | 0 | 0 |
| 56 | XM | 1 | 0 | 0 | 0 | 0 |
| 56 | XQ | 1 | 0 | 0 | 0 | 0 |
| 56 | XS | 1 | 0 | 0 | 0 | 0 |
| 56 | XV | 6 | 0 | 0 | 0 | 0 |
| 56 | Y0 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y7 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y8 | 1 | 0 | 0 | 0 | 0 |
| 56 | Y9 | 1 | 0 | 0 | 0 | 0 |
| 56 | YA | 546 | 0 | 0 | 0 | 0 |
| 56 | YB | 12 | 0 | 0 | 0 | 0 |
| 56 | YD | 2 | 0 | 0 | 0 | 0 |
| 56 | YE | 2 | 0 | 0 | 0 | 0 |
| 56 | YO | 1 | 0 | 0 | 0 | 0 |
| 56 | YP | 3 | 0 | 0 | 0 | 0 |
| 56 | YQ | 3 | 0 | 0 | 0 | 0 |
| 56 | YX | 2 | 0 | 0 | 0 | 0 |
| 56 | YY | 1 | 0 | 0 | 0 | 0 |
| 57 | QD | 8 | 0 | 0 | 1 | 0 |
| 57 | XD | 8 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58 | QN | 1 | 0 | 0 | 0 | 0 |
| 58 | R4 | 1 | 0 | 0 | 0 | 0 |
| 58 | R5 | 1 | 0 | 0 | 0 | 0 |
| 58 | R6 | 1 | 0 | 0 | 0 | 0 |
| 58 | R9 | 1 | 0 | 0 | 0 | 0 |
| 58 | RY | 1 | 0 | 0 | 0 | 0 |
| 58 | XN | 1 | 0 | 0 | 0 | 0 |
| 58 | Y4 | 1 | 0 | 0 | 0 | 0 |
| 58 | Y5 | 1 | 0 | 0 | 0 | 0 |
| 58 | Y6 | 1 | 0 | 0 | 0 | 0 |
| 58 | Y9 | 1 | 0 | 0 | 0 | 0 |
| 58 | YY | 1 | 0 | 0 | 0 | 0 |
| All | All | 295575 | 0 | 199664 | 5705 | 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 12.

All (5705) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:QD:119:GLN:CB | 4:QD:119:GLN:CG | 1.78 | 1.55 |
| 25:YA:2755:C:H42 | 55:Y9:1:MET:HG2 | 1.08 | 1.16 |
| 25:RA:2747:G:N2 | 25:RA:2757:A:H62 | 1.43 | 1.15 |
| 25:YA:2742:C:H1' | 55:Y9:26:ILE:HA | 1.33 | 1.10 |
| 25:RA:2747:G:H21 | 25:RA:2757:A:N6 | 1.52 | 1.05 |
| 10:QJ:26:ALA:HB1 | 10:QJ:84:GLN:HE21 | 1.19 | 1.04 |
| 27:RD:35:LYS:HB3 | 27:RD:36:PRO:HD2 | 1.42 | 1.02 |
| 25:YA:2867:G:HO2' | 25:YA:2868:A:H8 | 1.05 | 1.02 |
| 25:YA:2743:C:O5' | 55:Y9:26:ILE:N | 1.94 | 1.00 |
| 27:YD:35:LYS:HB3 | 27:YD:36:PRO:HD2 | 1.42 | 0.98 |
| 25:YA:2755:C:N4 | 55:Y9:1:MET:HG2 | 1.80 | 0.97 |
| 25:YA:2524:G:N2 | 55:Y9:29:ASN:OD1 | 1.99 | 0.96 |
| 22:XW:35:C:N4 | 23:XX:14:A:C6 | 2.34 | 0.94 |
| 25:RA:1464:C:HO2' | 25:RA:1528:A:H8 | 1.11 | 0.94 |
| 10:QJ:26:ALA:HB1 | 10:QJ:84:GLN:NE2 | 1.85 | 0.91 |
| 25:RA:2701:C:H3' | 25:RA:2702:U:H5'' | 1.52 | 0.90 |
| 25:YA:1568:G:H5'' | 27:YD:61:LEU:HD23 | 1.53 | 0.90 |
| 22:XW:35:C:N4 | 23:XX:14:A:N6 | 2.20 | 0.90 |
| 25:YA:2525:G:H21 | 55:Y9:28:GLU:HG3 | 1.37 | 0.90 |
| 25:YA:2526:G:H1 | 25:YA:2537:U:H3 | 0.94 | 0.89 |
| 27:YD:17:THR:HB | 27:YD:205:VAL:H | 1.38 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:QW:20:G:O6 | 25:RA:2112:G:N1 | 2.06 | 0.89 |
| 3:QC:20:SER:HB2 | 3:QC:40:ARG:HH22 | 1.36 | 0.87 |
| 31:RH:8:PRO:HG2 | 31:RH:69:ARG:HE | 1.38 | 0.87 |
| 5:XE:50:GLU:HG3 | 5:XE:52:PRO:HD2 | 1.54 | 0.87 |
| 3:XC:20:SER:HB2 | 3:XC:40:ARG:HH22 | 1.40 | 0.87 |
| 1:QA:1422:G:H5' | 34:RO:48:PRO:HB3 | 1.58 | 0.86 |
| 25:YA:888:C:H3' | 25:YA:889:C:H4' | 1.55 | 0.86 |
| 1:QA:827:U:O2 | 1:QA:874:G:N2 | 2.09 | 0.85 |
| 1:XA:689:C:H3' | 1:XA:690:G:H21 | 1.41 | 0.85 |
| 25:RA:1111:A:H5' | 31:RH:3:ARG:HH21 | 1.39 | 0.85 |
| 47:R1:87:PRO:HA | 47:R1:90:ILE:HG22 | 1.59 | 0.84 |
| 31:YH:87:LEU:HA | 55:Y9:18:ARG:HH22 | 1.41 | 0.84 |
| 31:YH:8:PRO:HG2 | 31:YH:69:ARG:HE | 1.41 | 0.84 |
| 25:RA:2049:G:N2 | 25:RA:2619:C:O2 | 2.09 | 0.83 |
| 25:YA:2539:C:O2 | 55:Y9:29:ASN:ND2 | 2.10 | 0.83 |
| 25:YA:996:A:OP2 | 40:YU:92:ARG:NH2 | 2.12 | 0.83 |
| 25:YA:2525:G:N3 | 55:Y9:28:GLU:HB2 | 1.92 | 0.83 |
| 25:YA:2745:C:H4' | 31:YH:142:GLY:HA3 | 1.61 | 0.82 |
| 25:YA:857:C:OP2 | 46:Y0:77:ARG:NH2 | 2.11 | 0.82 |
| 45:YZ:52:SER:O | 45:YZ:54:HIS:N | 2.12 | 0.82 |
| 19:QS:3:ARG:HE | 19:QS:7:LYS:HE2 | 1.42 | 0.82 |
| 25:RA:2789:C:O2 | 25:RA:2894:G:N2 | 2.12 | 0.82 |
| 25:RA:2882:A:OP1 | 37:RR:96:ARG:NH1 | 2.13 | 0.82 |
| 26:RB:33:G:OP2 | 30:RG:96:ARG:NH2 | 2.12 | 0.82 |
| 45:RZ:52:SER:O | 45:RZ:54:HIS:N | 2.13 | 0.82 |
| 25:YA:2470:G:H5' | 36:YQ:56:ARG:HH21 | 1.43 | 0.82 |
| 12:QL:117:ARG:HB2 | 12:QL:122:THR:HB | 1.59 | 0.82 |
| 26:RB:75:G:HO2' | 45:RZ:85:HIS:HE2 | 1.25 | 0.81 |
| 1:XA:403:C:OP2 | 4:XD:74:GLN:NE2 | 2.13 | 0.81 |
| 1:XA:1130:A:O2' | 9:XI:3:GLN:NE2 | 2.13 | 0.81 |
| 25:RA:2789:C:N3 | 25:RA:2894:G:N1 | 2.25 | 0.81 |
| 30:RG:29:TRP:O | 30:RG:33:ARG:NH1 | 2.14 | 0.81 |
| 25:YA:460:A:H62 | 25:YA:469:G:H21 | 1.29 | 0.81 |
| 1:QA:687:A:N6 | 1:QA:703:G:N2 | 2.29 | 0.81 |
| 4:QD:119:GLN:CD | 4:QD:119:GLN:CB | 2.48 | 0.81 |
| 2:XB:185:ILE:HG22 | 2:XB:199:TYR:HB2 | 1.62 | 0.81 |
| 45:YZ:7:ALA:HB2 | 45:YZ:59:LEU:HB3 | 1.63 | 0.81 |
| 45:RZ:166:SER:HB2 | 45:RZ:168:GLU:N | 1.96 | 0.80 |
| 16:XP:4:ILE:HG12 | 16:XP:21:VAL:HG12 | 1.61 | 0.80 |
| 25:RA:1030:G:O6 | 25:RA:1125:G:N2 | 2.14 | 0.80 |
| 30:YG:29:TRP:O | 30:YG:33:ARG:NH1 | 2.14 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:RN:133:GLN:HG2 | 33:RN:135:PRO:HD3 | 1.63 | 0.80 |
| 25:RA:140:A:H8 | 25:RA:1408:C:HO2' | 1.28 | 0.80 |
| 1:QA:687:A:H62 | 1:QA:703:G:N2 | 1.80 | 0.79 |
| 25:YA:2755:C:N4 | 55:Y9:2:LYS:O | 2.15 | 0.79 |
| 54:R8:29:LYS:HG3 | 54:R8:30:ARG:H | 1.47 | 0.79 |
| 54:Y8:29:LYS:HG3 | 54:Y8:30:ARG:H | 1.48 | 0.79 |
| 1:XA:1304:G:N2 | 1:XA:1334:G:O6 | 2.16 | 0.79 |
| 1:XA:376:G:H5'' | 16:XP:5:ARG:HB2 | 1.64 | 0.79 |
| 45:YZ:166:SER:HB2 | 45:YZ:168:GLU:N | 1.98 | 0.79 |
| 28:RE:17:ASP:O | 28:RE:19:ARG:N | 2.16 | 0.79 |
| 40:YU:92:ARG:HD2 | 41:YV:11:GLN:HB2 | 1.64 | 0.79 |
| 19:QS:18:LYS:HG2 | 19:QS:31:ILE:HD12 | 1.65 | 0.79 |
| 27:RD:17:THR:HB | 27:RD:205:VAL:H | 1.46 | 0.79 |
| 25:YA:67:U:H3 | 25:YA:74:A:H2 | 1.31 | 0.79 |
| 1:XA:950:U:H3 | 1:XA:1231:G:H1 | 1.30 | 0.78 |
| 1:QA:1351:U:H3 | 1:QA:1371:G:H1 | 1.30 | 0.78 |
| 25:YA:2746:U:O4 | 25:YA:2755:C:O2' | 2.01 | 0.78 |
| 25:YA:2882:A:OP1 | 37:YR:96:ARG:NH1 | 2.17 | 0.78 |
| 34:YO:104:ARG:HH21 | 39:YT:34:VAL:HG21 | 1.48 | 0.78 |
| 16:QP:4:ILE:HG12 | 16:QP:21:VAL:HG12 | 1.64 | 0.78 |
| 28:YE:17:ASP:O | 28:YE:19:ARG:N | 2.16 | 0.78 |
| 1:QA:618:C:H5' | 1:QA:619:U:H5'' | 1.64 | 0.78 |
| 1:XA:1086:U:H3 | 1:XA:1099:G:H22 | 1.31 | 0.78 |
| 35:YP:95:VAL:HG13 | 35:YP:100:LEU:HD21 | 1.66 | 0.78 |
| 40:RU:92:ARG:HD2 | 41:RV:11:GLN:HB2 | 1.67 | 0.77 |
| 45:RZ:7:ALA:HB2 | 45:RZ:59:LEU:HB3 | 1.66 | 0.77 |
| 6:QF:37:VAL:HA | 6:QF:65:VAL:HG12 | 1.66 | 0.77 |
| 1:XA:27:G:H4' | 4:XD:209:ARG:HG3 | 1.66 | 0.77 |
| 11:XK:83:ILE:HG12 | 11:XK:109:VAL:HB | 1.67 | 0.77 |
| 32:RI:88:ILE:HB | 32:RI:121:LYS:HG3 | 1.66 | 0.77 |
| 1:XA:1492:A:H5'' | 12:XL:47:LYS:HB3 | 1.66 | 0.77 |
| 33:YN:133:GLN:HG2 | 33:YN:135:PRO:HD3 | 1.67 | 0.77 |
| 25:RA:2527:C:H4' | 55:R9:4:ARG:HD3 | 1.66 | 0.77 |
| 35:RP:95:VAL:HG13 | 35:RP:100:LEU:HD21 | 1.66 | 0.77 |
| 26:YB:9:G:OP1 | 38:YS:15:ARG:NH1 | 2.16 | 0.77 |
| 25:YA:2495:G:H5'' | 36:YQ:81:VAL:HG12 | 1.67 | 0.77 |
| 25:RA:631:A:OP1 | 54:R8:46:ARG:NH2 | 2.18 | 0.77 |
| 38:RS:85:VAL:HG22 | 38:RS:110:LEU:HD22 | 1.66 | 0.77 |
| 1:XA:380:G:N2 | 1:XA:383:A:OP2 | 2.19 | 0.76 |
| 39:YT:62:THR:HG22 | 39:YT:75:ILE:HG12 | 1.67 | 0.76 |
| 39:YT:50:ILE:HD11 | 39:YT:100:TYR:HA | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:RD:13:ARG:NH1 | 27:RD:16:MET:SD | 2.58 | 0.76 |
| 25:YA:2741:A:C4 | 55:Y9:30:PRO:HD2 | 2.20 | 0.76 |
| 26:YB:33:G:H5' | 30:YG:2:PRO:HG3 | 1.66 | 0.76 |
| 1:QA:954:G:H21 | 1:QA:1227:A:H62 | 1.31 | 0.76 |
| 12:QL:104:VAL:HG12 | 12:QL:105:TYR:H | 1.50 | 0.76 |
| 36:RQ:81:VAL:O | 36:RQ:82:ARG:NE | 2.19 | 0.76 |
| 27:YD:8:PRO:HB3 | 27:YD:14:ARG:HB3 | 1.67 | 0.76 |
| 25:YA:958:U:OP2 | 36:YQ:14:ARG:NH1 | 2.18 | 0.76 |
| 36:YQ:60:ARG:HH11 | 45:YZ:113:ALA:HB3 | 1.51 | 0.76 |
| 28:RE:5:LEU:HG | 28:RE:49:LEU:HD23 | 1.68 | 0.76 |
| 25:YA:2741:A:O3' | 55:Y9:31:LYS:HB2 | 1.85 | 0.76 |
| 25:YA:879:G:N2 | 25:YA:898:C:O2 | 2.13 | 0.75 |
| 1:XA:8:A:N6 | 4:XD:205:GLU:O | 2.20 | 0.75 |
| 25:YA:2744:G:H5'' | 55:Y9:24:TYR:HB2 | 1.69 | 0.75 |
| 1:QA:689:C:H3' | 1:QA:690:G:H21 | 1.51 | 0.75 |
| 55:Y9:1:MET:HG3 | 55:Y9:33:LYS:HD2 | 1.67 | 0.75 |
| 25:YA:2526:G:H1' | 55:Y9:28:GLU:HB3 | 1.67 | 0.75 |
| 5:QE:50:GLU:HG3 | 5:QE:52:PRO:HD2 | 1.66 | 0.75 |
| 25:RA:1309:G:H4' | 53:R7:7:PRO:HB2 | 1.67 | 0.75 |
| 25:YA:2068:U:H3 | 25:YA:2430:A:H2 | 1.32 | 0.75 |
| 31:RH:164:TYR:HB2 | 31:RH:167:GLU:HB2 | 1.69 | 0.75 |
| 31:YH:89:ILE:HA | 31:YH:162:ILE:HG23 | 1.69 | 0.75 |
| 25:RA:1980:G:O2' | 25:RA:1982:C:OP2 | 2.05 | 0.75 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:H8 | 1.52 | 0.75 |
| 22:XW:35:C:C4 | 23:XX:14:A:N6 | 2.55 | 0.75 |
| 25:RA:2115:G:N2 | 25:RA:2165:G:N7 | 2.33 | 0.74 |
| 1:XA:1159:U:O2' | 1:XA:1160:G:N7 | 2.20 | 0.74 |
| 25:YA:589:C:H2' | 25:YA:590:A:H8 | 1.51 | 0.74 |
| 41:YV:43:GLU:HG3 | 41:YV:44:LYS:H | 1.51 | 0.74 |
| 30:RG:47:LYS:HD3 | 30:RG:81:LYS:HB2 | 1.67 | 0.74 |
| 25:YA:1359:A:H62 | 25:YA:1372:U:H3 | 1.34 | 0.74 |
| 27:RD:31:LYS:HB3 | 27:RD:35:LYS:HG3 | 1.70 | 0.74 |
| 27:YD:13:ARG:NH1 | 27:YD:16:MET:SD | 2.60 | 0.74 |
| 1:QA:664:G:H22 | 1:QA:741:G:H1 | 1.34 | 0.74 |
| 1:QA:842:C:O2' | 1:QA:848:C:N4 | 2.20 | 0.74 |
| 50:Y4:56:VAL:HG23 | 50:Y4:58:ARG:HG3 | 1.69 | 0.74 |
| 31:YH:149:ARG:HE | 55:Y9:20:HIS:H | 1.33 | 0.74 |
| 1:XA:1123:A:H4' | 10:XJ:36:GLY:HA3 | 1.66 | 0.74 |
| 27:RD:8:PRO:HB3 | 27:RD:14:ARG:HB3 | 1.70 | 0.74 |
| 11:QK:58:PRO:HB2 | 11:QK:93:GLN:HG3 | 1.67 | 0.73 |
| 43:YX:54:VAL:HG22 | 43:YX:81:VAL:HG23 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1165:U:H3 | 25:RA:1184:G:H1 | 1.33 | 0.73 |
| 25:RA:2328:A:H2' | 25:RA:2329:G:C8 | 2.24 | 0.73 |
| 25:YA:2741:A:H2' | 55:Y9:29:ASN:CG | 2.09 | 0.73 |
| 28:RE:10:GLY:HA3 | 39:RT:8:LYS:HD3 | 1.69 | 0.73 |
| 2:QB:185:ILE:HG22 | 2:QB:199:TYR:HB2 | 1.69 | 0.73 |
| 27:RD:71:ASP:HB2 | 27:RD:103:ARG:HH12 | 1.51 | 0.73 |
| 27:RD:182:LEU:H | 27:RD:272:ALA:HB3 | 1.54 | 0.73 |
| 22:XW:8:U:N3 | 22:XW:14:A:C8 | 2.57 | 0.73 |
| 55:Y9:1:MET:HG3 | 55:Y9:33:LYS:HB3 | 1.71 | 0.73 |
| 25:YA:2701:C:H3' | 25:YA:2702:U:H5'' | 1.68 | 0.73 |
| 41:RV:43:GLU:HG3 | 41:RV:44:LYS:H | 1.53 | 0.73 |
| 34:YO:104:ARG:NH2 | 39:YT:43:GLN:OE1 | 2.21 | 0.73 |
| 1:XA:674:G:H2' | 1:XA:675:A:H8 | 1.53 | 0.73 |
| 25:YA:2755:C:C5 | 55:Y9:35:ARG:HB3 | 2.24 | 0.73 |
| 1:QA:1238:A:OP1 | 1:QA:1335:C:O2' | 2.07 | 0.73 |
| 38:YS:85:VAL:HG22 | 38:YS:110:LEU:HD22 | 1.68 | 0.73 |
| 1:QA:1492:A:H5'' | 12:QL:47:LYS:HB3 | 1.69 | 0.73 |
| 22:QW:8:U:N3 | 22:QW:14:A:C8 | 2.56 | 0.73 |
| 25:YA:2814:C:HO2' | 51:Y5:29:THR:HG1 | 1.35 | 0.73 |
| 28:YE:76:ARG:HD3 | 28:YE:195:LEU:HD22 | 1.71 | 0.73 |
| 25:YA:2744:G:N2 | 31:YH:143:GLN:OE1 | 2.22 | 0.73 |
| 25:YA:2246:G:H2' | 25:YA:2247:A:H8 | 1.54 | 0.72 |
| 25:RA:593:G:H4' | 54:R8:61:LEU:HD13 | 1.70 | 0.72 |
| 1:QA:452:A:H62 | 1:QA:480:U:H3 | 1.35 | 0.72 |
| 47:Y1:80:LEU:HD12 | 47:Y1:81:LYS:HG2 | 1.71 | 0.72 |
| 25:YA:1309:G:H4' | 53:Y7:7:PRO:HB2 | 1.71 | 0.72 |
| 25:YA:2742:C:C2 | 55:Y9:30:PRO:HA | 2.25 | 0.72 |
| 31:YH:46:GLU:OE1 | 31:YH:51:ARG:NH1 | 2.21 | 0.72 |
| 25:RA:17:G:H4' | 40:RU:25:TRP:HE1 | 1.55 | 0.72 |
| 1:XA:1422:G:H5'' | 34:YO:48:PRO:HB3 | 1.71 | 0.72 |
| 1:QA:687:A:N6 | 1:QA:703:G:H21 | 1.87 | 0.72 |
| 1:QA:953:G:H5' | 1:QA:965:A:H61 | 1.55 | 0.72 |
| 35:RP:101:VAL:HB | 35:RP:106:LEU:HB2 | 1.71 | 0.72 |
| 39:RT:39:ARG:HH22 | 39:RT:41:ARG:HD3 | 1.54 | 0.72 |
| 25:YA:2572:A:H2' | 28:YE:144:ARG:HD3 | 1.71 | 0.72 |
| 25:YA:2784:C:O2' | 28:YE:37:ARG:NH1 | 2.21 | 0.72 |
| 39:RT:50:ILE:HD11 | 39:RT:100:TYR:HA | 1.69 | 0.72 |
| 25:RA:2784:C:O2' | 28:RE:37:ARG:NH1 | 2.23 | 0.72 |
| 25:YA:2739:U:H2' | 25:YA:2740:A:C8 | 2.24 | 0.72 |
| 25:YA:1403:C:H5'' | 25:YA:1471:A:H1' | 1.71 | 0.72 |
| 25:RA:2502:G:H5'' | 25:RA:2503:A:H5'' | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:YH:86:GLU:HG3 | 31:YH:164:TYR:HD1 | 1.55 | 0.72 |
| 39:RT:66:VAL:HA | 39:RT:71:GLY:HA2 | 1.72 | 0.71 |
| 1:XA:1348:U:H3 | 1:XA:1374:A:H2 | 1.37 | 0.71 |
| 25:YA:17:G:H4' | 40:YU:25:TRP:HE1 | 1.53 | 0.71 |
| 1:XA:1137:C:O2' | 1:XA:1138:G:N2 | 2.22 | 0.71 |
| 1:XA:278:G:OP2 | 17:XQ:92:ARG:NH2 | 2.23 | 0.71 |
| 1:XA:448:A:OP2 | 1:XA:485:G:N2 | 2.22 | 0.71 |
| 1:XA:1227:A:OP1 | 19:XS:80:TYR:OH | 2.07 | 0.71 |
| 1:QA:713:G:H2' | 1:QA:714:G:C8 | 2.26 | 0.71 |
| 25:RA:1600:C:OP1 | 43:RX:58:HIS:NE2 | 2.19 | 0.71 |
| 28:RE:9:VAL:HB | 28:RE:25:VAL:HG23 | 1.72 | 0.71 |
| 22:QV:59:A:O2' | 22:QV:61:U:OP2 | 2.07 | 0.71 |
| 22:QW:20:G:O6 | 25:RA:2112:G:N2 | 2.24 | 0.71 |
| 25:RA:993:G:OP1 | 40:RU:50:ARG:NH2 | 2.23 | 0.71 |
| 45:RZ:163:LEU:HD13 | 45:RZ:167:PRO:HD3 | 1.72 | 0.71 |
| 25:YA:2743:C:O2' | 25:YA:2744:G:H5'' | 1.91 | 0.71 |
| 27:RD:151:LYS:O | 27:RD:154:LYS:NZ | 2.23 | 0.71 |
| 25:YA:2328:A:H2' | 25:YA:2329:G:C8 | 2.25 | 0.71 |
| 25:YA:265:A:N6 | 25:YA:427:U:O2' | 2.23 | 0.71 |
| 32:YI:88:ILE:HB | 32:YI:121:LYS:HG3 | 1.72 | 0.71 |
| 35:YP:135:LEU:HG | 35:YP:139:LYS:HE2 | 1.71 | 0.71 |
| 36:YQ:81:VAL:O | 36:YQ:82:ARG:NE | 2.23 | 0.71 |
| 1:QA:1249:C:O2' | 9:QI:73:GLN:NE2 | 2.24 | 0.71 |
| 1:QA:1266:G:N2 | 1:QA:1269:A:OP2 | 2.24 | 0.71 |
| 25:YA:2540:C:H1' | 25:YA:2741:A:N3 | 2.05 | 0.71 |
| 1:QA:714:G:H2' | 1:QA:715:A:C8 | 2.25 | 0.71 |
| 25:RA:1800:C:OP2 | 27:RD:183:ARG:NH1 | 2.22 | 0.71 |
| 27:YD:36:PRO:HA | 27:YD:62:TYR:O | 1.90 | 0.71 |
| 28:YE:31:CYS:HB3 | 28:YE:49:LEU:HG | 1.71 | 0.71 |
| 4:QD:62:GLN:HE22 | 4:QD:65:ARG:HH21 | 1.38 | 0.71 |
| 7:QG:84:ASN:ND2 | 22:QW:34:U:OP1 | 2.23 | 0.71 |
| 28:RE:31:CYS:HB3 | 28:RE:49:LEU:HG | 1.73 | 0.71 |
| 54:Y8:29:LYS:O | 54:Y8:31:HIS:N | 2.24 | 0.71 |
| 2:QB:80:ILE:HD11 | 2:QB:208:ILE:HG23 | 1.72 | 0.71 |
| 25:YA:2525:G:H4' | 55:Y9:28:GLU:HA | 1.71 | 0.71 |
| 27:YD:31:LYS:HB3 | 27:YD:35:LYS:HG3 | 1.71 | 0.71 |
| 27:RD:132:PRO:HG3 | 27:RD:190:TYR:HE1 | 1.56 | 0.70 |
| 39:RT:62:THR:HG22 | 39:RT:75:ILE:HG12 | 1.72 | 0.70 |
| 25:RA:996:A:OP2 | 40:RU:92:ARG:NH2 | 2.23 | 0.70 |
| 34:RO:104:ARG:HH21 | 39:RT:34:VAL:HG21 | 1.54 | 0.70 |
| 1:XA:714:G:H2' | 1:XA:715:A:C8 | 2.26 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:690:G:H22 | 11:QK:55:LYS:HZ1 | 1.39 | 0.70 |
| 27:RD:24:ILE:HD11 | 27:RD:91:ARG:HD2 | 1.72 | 0.70 |
| 25:YA:2526:G:O6 | 25:YA:2537:U:O4 | 2.09 | 0.70 |
| 31:RH:46:GLU:OE1 | 31:RH:51:ARG:NH1 | 2.25 | 0.70 |
| 55:Y9:22:ARG:HB2 | 55:Y9:24:TYR:HE2 | 1.57 | 0.70 |
| 25:YA:2666:C:O2 | 31:YH:152:ARG:NH1 | 2.24 | 0.70 |
| 34:RO:104:ARG:NH2 | 39:RT:43:GLN:OE1 | 2.25 | 0.70 |
| 1:XA:842:C:O2' | 1:XA:848:C:N4 | 2.25 | 0.70 |
| 1:XA:1347:G:N2 | 1:XA:1374:A:OP2 | 2.24 | 0.70 |
| 2:XB:80:ILE:HD11 | 2:XB:208:ILE:HG23 | 1.74 | 0.70 |
| 48:R2:22:GLU:OE2 | 48:R2:68:ARG:NH2 | 2.25 | 0.70 |
| 1:XA:544:G:OP1 | 4:XD:59:ARG:NH2 | 2.24 | 0.70 |
| 1:XA:673:G:H2' | 1:XA:674:G:C8 | 2.27 | 0.70 |
| 25:YA:1817:G:OP1 | 27:YD:88:ARG:NH2 | 2.24 | 0.70 |
| 1:QA:8:A:N6 | 4:QD:205:GLU:O | 2.25 | 0.70 |
| 4:QD:30:LYS:HG2 | 4:QD:35:ARG:HH21 | 1.56 | 0.70 |
| 10:QJ:49:VAL:HG13 | 14:QN:41:ARG:HB2 | 1.74 | 0.70 |
| 18:QR:86:VAL:HG12 | 18:QR:87:ARG:HG2 | 1.74 | 0.70 |
| 1:XA:1023:G:H3' | 1:XA:1024:G:H5'' | 1.73 | 0.70 |
| 27:YD:168:ARG:HG2 | 27:YD:173:VAL:HG12 | 1.74 | 0.70 |
| 33:YN:54:VAL:HB | 33:YN:122:VAL:HG22 | 1.73 | 0.70 |
| 38:YS:20:ARG:NH1 | 46:Y0:48:GLY:O | 2.25 | 0.70 |
| 6:QF:68:PRO:HG3 | 6:QF:71:ARG:HH21 | 1.57 | 0.69 |
| 45:RZ:4:ARG:HG2 | 45:RZ:58:VAL:HB | 1.72 | 0.69 |
| 1:XA:992:U:H3 | 1:XA:1044:A:H62 | 1.39 | 0.69 |
| 1:XA:31:G:O2' | 1:XA:48:C:N4 | 2.24 | 0.69 |
| 28:YE:5:LEU:HG | 28:YE:49:LEU:HD23 | 1.71 | 0.69 |
| 1:QA:1306:A:N6 | 1:QA:1331:G:O2' | 2.25 | 0.69 |
| 54:R8:29:LYS:O | 54:R8:31:HIS:N | 2.24 | 0.69 |
| 47:Y1:87:PRO:HA | 47:Y1:90:ILE:HG22 | 1.75 | 0.69 |
| 53:Y7:10:ARG:HE | 53:Y7:14:LYS:HD2 | 1.57 | 0.69 |
| 1:QA:1356:G:H2' | 1:QA:1357:A:C8 | 2.27 | 0.69 |
| 46:R0:27:GLU:HG3 | 46:R0:68:GLU:HA | 1.74 | 0.69 |
| 22:QW:20:G:O6 | 25:RA:2112:G:C2 | 2.45 | 0.69 |
| 41:RV:24:LYS:HA | 41:RV:92:THR:HG23 | 1.75 | 0.69 |
| 18:XR:86:VAL:HG12 | 18:XR:87:ARG:HG2 | 1.72 | 0.69 |
| 25:YA:2743:C:O2 | 55:Y9:19:ARG:NH1 | 2.25 | 0.69 |
| 45:RZ:5:LEU:H | 45:RZ:59:LEU:HA | 1.56 | 0.69 |
| 10:XJ:38:ILE:HD11 | 10:XJ:71:LEU:HD23 | 1.75 | 0.69 |
| 25:YA:2742:C:C5 | 55:Y9:33:LYS:HB2 | 2.27 | 0.69 |
| 25:RA:1649:G:O2' | 37:RR:107:ASP:OD1 | 2.05 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:YP:101:VAL:HG21 | 35:YP:108:LYS:HD2 | 1.74 | 0.69 |
| 40:YU:85:LYS:NZ | 40:YU:117:GLN:OE1 | 2.26 | 0.69 |
| 4:QD:119:GLN:CA | 4:QD:119:GLN:CG | 2.69 | 0.69 |
| 1:QA:1130:A:O2' | 9:QI:3:GLN:NE2 | 2.26 | 0.69 |
| 25:RA:1857:G:H21 | 25:RA:1886:C:H42 | 1.40 | 0.69 |
| 25:RA:2584:U:H2' | 25:RA:2585:U:H2' | 1.73 | 0.69 |
| 1:XA:811:C:O2' | 1:XA:901:A:N1 | 2.25 | 0.69 |
| 48:Y2:22:GLU:OE2 | 48:Y2:68:ARG:NH2 | 2.26 | 0.69 |
| 45:YZ:163:LEU:HD13 | 45:YZ:167:PRO:HD3 | 1.74 | 0.69 |
| 1:QA:1009:G:H1 | 1:QA:1020:U:H3 | 1.41 | 0.69 |
| 45:YZ:4:ARG:HG2 | 45:YZ:58:VAL:HB | 1.74 | 0.69 |
| 2:QB:84:GLU:HB3 | 2:QB:219:VAL:HG21 | 1.75 | 0.69 |
| 47:R1:80:LEU:HD12 | 47:R1:81:LYS:HG2 | 1.74 | 0.69 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:HE2 | 1.58 | 0.69 |
| 25:RA:2308:G:H22 | 25:RA:2311:A:H2 | 1.40 | 0.69 |
| 37:RR:104:ARG:HG3 | 37:RR:107:ASP:HB3 | 1.75 | 0.69 |
| 25:YA:2023:G:H5' | 25:YA:2617:C:H4' | 1.74 | 0.69 |
| 27:YD:132:PRO:HG3 | 27:YD:190:TYR:HE1 | 1.58 | 0.69 |
| 28:YE:9:VAL:HB | 28:YE:25:VAL:HG23 | 1.74 | 0.69 |
| 30:YG:5:VAL:HG11 | 30:YG:100:TRP:HB3 | 1.75 | 0.69 |
| 43:YX:53:LYS:NZ | 43:YX:55:ASN:OD1 | 2.26 | 0.69 |
| 1:QA:1023:G:H3' | 1:QA:1024:G:H5'' | 1.75 | 0.69 |
| 3:QC:150:LYS:HE3 | 3:QC:167:TRP:HE1 | 1.58 | 0.69 |
| 25:RA:141:A:H8 | 25:RA:1595:G:H21 | 1.41 | 0.69 |
| 25:RA:1678:G:H22 | 25:RA:1989:G:H22 | 1.38 | 0.69 |
| 1:QA:1347:G:N2 | 1:QA:1374:A:OP2 | 2.23 | 0.69 |
| 47:R1:76:ARG:HH11 | 47:R1:94:LEU:HD13 | 1.58 | 0.69 |
| 4:XD:13:ARG:HH21 | 4:XD:40:PRO:HB3 | 1.58 | 0.69 |
| 25:RA:252:G:OP2 | 35:RP:50:ARG:NH1 | 2.26 | 0.68 |
| 1:XA:789:U:H1' | 1:XA:792:A:H2 | 1.57 | 0.68 |
| 1:XA:80:G:H1 | 1:XA:89:U:H3 | 1.38 | 0.68 |
| 25:YA:630:G:N2 | 25:YA:633:A:OP2 | 2.22 | 0.68 |
| 45:YZ:53:ILE:HG22 | 45:YZ:71:VAL:HG13 | 1.75 | 0.68 |
| 19:QS:12:ASP:OD2 | 19:QS:35:SER:OG | 2.11 | 0.68 |
| 25:RA:911:A:H2' | 36:RQ:9:TYR:HE2 | 1.58 | 0.68 |
| 25:RA:2701:C:H3' | 25:RA:2702:U:C5' | 2.22 | 0.68 |
| 29:RF:63:LYS:HE2 | 29:RF:67:GLN:HB2 | 1.73 | 0.68 |
| 1:XA:377:G:H2' | 1:XA:378:G:C8 | 2.27 | 0.68 |
| 25:YA:577:G:O2' | 25:YA:1254:A:OP1 | 2.12 | 0.68 |
| 25:YA:820:A:N3 | 25:YA:943:U:O2' | 2.26 | 0.68 |
| 39:YT:39:ARG:HH22 | 39:YT:41:ARG:HD3 | 1.57 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:QA:806:C:H2' | 1:QA:807:A:H8 | 1.58 | 0.68 |
| 1:XA:1356:G:H2' | 1:XA:1357:A:C8 | 2.28 | 0.68 |
| 10:XJ:49:VAL:HG23 | 14:XN:41:ARG:HB2 | 1.74 | 0.68 |
| 55:Y9:28:GLU:HG2 | 55:Y9:29:ASN:HB2 | 1.75 | 0.68 |
| 25:YA:1992:G:H5' | 25:YA:1994:C:H41 | 1.58 | 0.68 |
| 25:YA:2246:G:H2' | 25:YA:2247:A:C8 | 2.27 | 0.68 |
| 36:YQ:43:THR:HG22 | 36:YQ:94:VAL:HG12 | 1.74 | 0.68 |
| 1:QA:1347:G:O6 | 9:QI:10:ARG:NH2 | 2.27 | 0.68 |
| 36:RQ:137:TYR:HB3 | 45:RZ:76:LEU:HD11 | 1.76 | 0.68 |
| 1:XA:1287:A:H2' | 1:XA:1288:A:C8 | 2.28 | 0.68 |
| 54:Y8:26:LYS:HD2 | 54:Y8:47:LYS:HD3 | 1.75 | 0.68 |
| 1:QA:448:A:OP2 | 1:QA:485:G:N2 | 2.27 | 0.68 |
| 31:RH:121:ILE:HG13 | 31:RH:144:VAL:HG21 | 1.76 | 0.68 |
| 45:RZ:166:SER:HB2 | 45:RZ:168:GLU:H | 1.57 | 0.68 |
| 25:YA:2111:C:N3 | 25:YA:2118:U:O2' | 2.27 | 0.68 |
| 25:YA:288:C:H2' | 25:YA:289:A:H8 | 1.59 | 0.68 |
| 25:YA:581:C:H2' | 25:YA:582:G:H8 | 1.59 | 0.68 |
| 25:RA:2328:A:H2' | 25:RA:2329:G:H8 | 1.56 | 0.68 |
| 31:RH:52:VAL:O | 31:RH:65:HIS:NE2 | 2.26 | 0.68 |
| 1:XA:1316:G:N2 | 1:XA:1319:A:OP2 | 2.26 | 0.68 |
| 6:XF:37:VAL:HA | 6:XF:65:VAL:HG12 | 1.74 | 0.68 |
| 25:YA:1021:A:H61 | 25:YA:1142(A):A:H61 | 1.41 | 0.68 |
| 25:YA:1230:C:H2' | 25:YA:1231:G:H8 | 1.59 | 0.68 |
| 25:YA:1657:C:H2' | 25:YA:1658:C:H6 | 1.58 | 0.68 |
| 25:YA:2328:A:H2' | 25:YA:2329:G:H8 | 1.58 | 0.68 |
| 1:QA:191:G:O2' | 20:QT:101:GLY:O | 2.11 | 0.68 |
| 17:XQ:9:VAL:HG22 | 17:XQ:56:VAL:HG22 | 1.76 | 0.68 |
| 30:YG:47:LYS:HD3 | 30:YG:81:LYS:HB2 | 1.75 | 0.68 |
| 25:RA:1059:G:O6 | 25:RA:1079:C:N4 | 2.26 | 0.68 |
| 26:RB:9:G:OP1 | 38:RS:15:ARG:NH1 | 2.23 | 0.68 |
| 47:Y1:18:ILE:HG12 | 47:Y1:37:ILE:HG12 | 1.76 | 0.68 |
| 36:YQ:66:ILE:HA | 36:YQ:104:PHE:HA | 1.76 | 0.68 |
| 1:QA:1055:A:N7 | 1:QA:1200:C:N4 | 2.42 | 0.67 |
| 13:QM:93:ARG:NH1 | 25:RA:888:C:OP1 | 2.28 | 0.67 |
| 25:RA:1365:A:O2' | 47:R1:11:ARG:NH2 | 2.26 | 0.67 |
| 25:RA:270:A:OP2 | 25:RA:270(Y):G:N1 | 2.27 | 0.67 |
| 36:RQ:75:THR:HG21 | 36:RQ:85:LYS:HE3 | 1.75 | 0.67 |
| 1:XA:269:C:H2' | 1:XA:270:A:H8 | 1.58 | 0.67 |
| 25:YA:1116:C:H2' | 25:YA:1117:G:H8 | 1.59 | 0.67 |
| 25:YA:1860:G:H1 | 25:YA:1882:C:H42 | 1.43 | 0.67 |
| 1:QA:851:G:H2' | 1:QA:852:G:H8 | 1.60 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:QI:112:LYS:HA | 9:QI:119:ALA:HB2 | 1.77 | 0.67 |
| 25:YA:330:A:H2 | 25:YA:1210:A:HO2' | 1.42 | 0.67 |
| 40:YU:91:ASP:HA | 40:YU:95:LEU:HB2 | 1.76 | 0.67 |
| 45:YZ:5:LEU:H | 45:YZ:59:LEU:HA | 1.59 | 0.67 |
| 1:QA:1162:C:H42 | 1:QA:1174:G:H1 | 1.42 | 0.67 |
| 38:YS:30:ARG:HD2 | 38:YS:97:ARG:HD3 | 1.77 | 0.67 |
| 30:RG:18:GLU:OE2 | 30:RG:21:ARG:NH2 | 2.25 | 0.67 |
| 33:RN:54:VAL:HB | 33:RN:122:VAL:HG22 | 1.74 | 0.67 |
| 1:XA:1178:G:N2 | 1:XA:1181:G:N7 | 2.43 | 0.67 |
| 1:XA:1298:C:H2' | 7:XG:114:ARG:HH12 | 1.59 | 0.67 |
| 16:XP:4:ILE:HB | 16:XP:66:PRO:HB3 | 1.75 | 0.67 |
| 25:YA:2199:A:OP1 | 47:Y1:50:ARG:NH2 | 2.27 | 0.67 |
| 1:QA:619:U:N3 | 4:QD:134:ASP:OD1 | 2.23 | 0.67 |
| 1:QA:28:G:OP1 | 4:QD:76:ARG:NH1 | 2.24 | 0.67 |
| 1:XA:639:G:H2' | 1:XA:640:A:H8 | 1.60 | 0.67 |
| 25:YA:1068:G:O2' | 25:YA:1096:A:N3 | 2.28 | 0.67 |
| 1:QA:685:G:H21 | 1:QA:706:A:N6 | 1.93 | 0.67 |
| 25:RA:814:C:H1' | 25:RA:1226:G:H21 | 1.59 | 0.67 |
| 45:RZ:13:GLU:HB3 | 45:RZ:18:LEU:HD11 | 1.76 | 0.67 |
| 25:YA:2526:G:H2' | 25:YA:2527:C:C5 | 2.30 | 0.67 |
| 1:QA:972:C:H4' | 10:QJ:57:LYS:HB2 | 1.77 | 0.67 |
| 29:RF:154:VAL:HG22 | 29:RF:191:ARG:HB3 | 1.77 | 0.67 |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HB2 | 1.77 | 0.67 |
| 31:YH:149:ARG:NE | 55:Y9:20:HIS:H | 1.93 | 0.67 |
| 25:YA:1651:G:OP1 | 37:YR:40:LYS:NZ | 2.25 | 0.67 |
| 29:YF:32:LEU:HD11 | 29:YF:105:VAL:HG13 | 1.76 | 0.67 |
| 36:YQ:24:GLY:H | 36:YQ:101:ARG:HD2 | 1.60 | 0.67 |
| 27:RD:94:LEU:HD13 | 27:RD:104:TYR:HE1 | 1.59 | 0.67 |
| 46:Y0:27:GLU:HG3 | 46:Y0:68:GLU:HA | 1.75 | 0.67 |
| 31:YH:164:TYR:HB2 | 31:YH:167:GLU:HB2 | 1.76 | 0.67 |
| 1:QA:973:G:H4' | 14:QN:41:ARG:HH22 | 1.60 | 0.67 |
| 25:RA:1817:G:OP1 | 27:RD:88:ARG:NH2 | 2.27 | 0.67 |
| 45:RZ:128:VAL:HG22 | 45:RZ:129:SER:H | 1.60 | 0.67 |
| 1:XA:1002:G:H2' | 1:XA:1003:G:H8 | 1.59 | 0.67 |
| 3:XC:150:LYS:HE3 | 3:XC:167:TRP:HE1 | 1.60 | 0.67 |
| 25:YA:2646:C:OP2 | 25:YA:2732:G:O2' | 2.11 | 0.67 |
| 45:YZ:166:SER:HB2 | 45:YZ:168:GLU:H | 1.59 | 0.67 |
| 1:QA:1043:C:H2' | 1:QA:1044:A:H8 | 1.60 | 0.67 |
| 18:QR:32:ARG:HA | 18:QR:69:THR:HG21 | 1.76 | 0.67 |
| 25:RA:958:U:OP2 | 36:RQ:14:ARG:NH1 | 2.28 | 0.67 |
| 27:RD:36:PRO:HA | 27:RD:62:TYR:O | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:YD:69:ARG:NH2 | 27:YD:128:GLY:O | 2.24 | 0.67 |
| 30:YG:18:GLU:OE2 | 30:YG:21:ARG:NH2 | 2.27 | 0.67 |
| 43:YX:26:TYR:HD2 | 43:YX:89:ILE:HD12 | 1.58 | 0.67 |
| 1:QA:335:C:H2' | 1:QA:336:C:H6 | 1.58 | 0.66 |
| 45:RZ:53:ILE:HG22 | 45:RZ:71:VAL:HG13 | 1.76 | 0.66 |
| 25:YA:1111:A:OP1 | 31:YH:3:ARG:NH2 | 2.28 | 0.66 |
| 25:YA:460:A:H62 | 25:YA:469:G:N2 | 1.91 | 0.66 |
| 25:RA:819:A:OP2 | 25:RA:1187:G:N2 | 2.26 | 0.66 |
| 25:YA:1800:C:OP2 | 27:YD:183:ARG:NH1 | 2.20 | 0.66 |
| 25:YA:662:G:OP1 | 35:YP:15:ARG:NH1 | 2.27 | 0.66 |
| 1:QA:544:G:OP1 | 4:QD:59:ARG:NH2 | 2.27 | 0.66 |
| 1:XA:1129:C:OP1 | 9:XI:62:TYR:OH | 2.13 | 0.66 |
| 25:YA:2185:C:H2' | 25:YA:2186:G:H8 | 1.60 | 0.66 |
| 25:RA:1341:U:OP2 | 25:RA:1394:U:O2' | 2.12 | 0.66 |
| 25:RA:1478:G:H2' | 25:RA:1479:G:H8 | 1.59 | 0.66 |
| 25:RA:2109:U:H2' | 25:RA:2110:G:C8 | 2.31 | 0.66 |
| 36:RQ:24:GLY:H | 36:RQ:101:ARG:HD2 | 1.59 | 0.66 |
| 11:XK:86:GLY:O | 11:XK:91:ARG:NH1 | 2.26 | 0.66 |
| 12:XL:77:LEU:HD21 | 12:XL:107:ALA:HB2 | 1.78 | 0.66 |
| 31:YH:52:VAL:O | 31:YH:65:HIS:NE2 | 2.28 | 0.66 |
| 1:QA:1356:G:H2' | 1:QA:1357:A:H8 | 1.59 | 0.66 |
| 1:QA:978:A:OP2 | 1:QA:1362(A):C:N4 | 2.27 | 0.66 |
| 1:QA:545:C:H5' | 4:QD:72:GLU:HG3 | 1.75 | 0.66 |
| 19:QS:40:ILE:HG13 | 19:QS:44:MET:HG3 | 1.78 | 0.66 |
| 25:RA:1542:G:O6 | 25:RA:1543:A:N6 | 2.29 | 0.66 |
| 25:RA:1902:C:OP1 | 27:RD:242:ARG:NH2 | 2.28 | 0.66 |
| 28:RE:201:THR:HG22 | 28:RE:203:LYS:H | 1.60 | 0.66 |
| 25:YA:1657:C:H2' | 25:YA:1658:C:C6 | 2.30 | 0.66 |
| 1:XA:279:A:OP2 | 17:XQ:95:TYR:OH | 2.12 | 0.66 |
| 1:XA:636:U:H2' | 1:XA:637:G:H8 | 1.60 | 0.66 |
| 1:XA:643:C:H2' | 1:XA:644:G:H8 | 1.61 | 0.66 |
| 1:QA:266:G:O2' | 1:QA:267:C:OP2 | 2.12 | 0.66 |
| 11:QK:18:ARG:HG2 | 11:QK:81:ASP:HB2 | 1.77 | 0.66 |
| 33:RN:99:LEU:HD12 | 33:RN:122:VAL:HG21 | 1.78 | 0.66 |
| 1:XA:972:C:OP2 | 10:XJ:57:LYS:NZ | 2.29 | 0.66 |
| 31:YH:162:ILE:HG22 | 55:Y9:18:ARG:HH12 | 1.61 | 0.66 |
| 25:YA:28:A:N6 | 25:YA:512:G:O2' | 2.28 | 0.66 |
| 50:R4:16:CYS:SG | 50:R4:17:GLY:N | 2.68 | 0.66 |
| 25:YA:2755:C:H5' | 55:Y9:3:VAL:HG13 | 1.76 | 0.66 |
| 40:YU:61:TRP:HB3 | 40:YU:93:LYS:O | 1.95 | 0.66 |
| 1:QA:323:U:OP1 | 20:QT:26:ASN:ND2 | 2.28 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:587:C:OP2 | 35:RP:21:ARG:NH1 | 2.29 | 0.66 |
| 28:RE:104:VAL:HG11 | 28:RE:188:VAL:HG23 | 1.78 | 0.66 |
| 1:XA:713:G:H2' | 1:XA:714:G:C8 | 2.30 | 0.66 |
| 1:QA:1071:C:H2' | 1:QA:1072:G:H8 | 1.60 | 0.66 |
| 2:QB:20:GLU:HG3 | 2:QB:191:ASP:HB2 | 1.77 | 0.66 |
| 19:QS:41:VAL:HG11 | 19:QS:67:VAL:HA | 1.78 | 0.66 |
| 25:RA:818:G:N1 | 25:RA:1188:U:OP2 | 2.19 | 0.66 |
| 1:XA:266:G:O2' | 1:XA:267:C:OP2 | 2.14 | 0.66 |
| 1:XA:715:A:H2' | 1:XA:716:A:C8 | 2.30 | 0.66 |
| 1:QA:537:G:H5'' | 12:QL:113:ARG:HH12 | 1.61 | 0.65 |
| 1:XA:426:G:OP1 | 4:XD:38:TYR:OH | 2.12 | 0.65 |
| 11:XK:54:ARG:NH2 | 22:XW:40:C:O2' | 2.29 | 0.65 |
| 25:RA:1568:G:H5'' | 27:RD:61:LEU:HD23 | 1.78 | 0.65 |
| 1:XA:545:C:H5' | 4:XD:72:GLU:HG3 | 1.78 | 0.65 |
| 22:XV:35:C:H2' | 22:XV:36:A:H8 | 1.60 | 0.65 |
| 25:YA:2525:G:O2' | 25:YA:2526:G:O4' | 2.14 | 0.65 |
| 41:YV:24:LYS:HA | 41:YV:92:THR:HG23 | 1.78 | 0.65 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:H | 1.61 | 0.65 |
| 1:XA:1095:U:OP1 | 1:XA:1108:G:N2 | 2.23 | 0.65 |
| 2:XB:47:THR:HA | 2:XB:202:PRO:HG2 | 1.78 | 0.65 |
| 25:YA:2739:U:H2' | 25:YA:2740:A:H8 | 1.58 | 0.65 |
| 1:QA:1348:U:H4' | 9:QI:120:ARG:HD2 | 1.79 | 0.65 |
| 25:RA:662:G:OP1 | 35:RP:15:ARG:NH1 | 2.30 | 0.65 |
| 35:YP:65:ARG:O | 35:YP:68:GLN:NE2 | 2.29 | 0.65 |
| 1:QA:1192:C:O2 | 5:QE:25:ARG:NH2 | 2.30 | 0.65 |
| 1:QA:976:G:N2 | 1:QA:1362(A):C:OP2 | 2.23 | 0.65 |
| 25:RA:1497:U:H5'' | 25:RA:1498:C:H5 | 1.61 | 0.65 |
| 25:RA:2495:G:H5'' | 36:RQ:81:VAL:HG12 | 1.79 | 0.65 |
| 25:YA:2788:C:O2' | 25:YA:2809:A:N3 | 2.28 | 0.65 |
| 25:YA:83:G:H1 | 25:YA:102:G:HO2' | 1.41 | 0.65 |
| 43:RX:26:TYR:HD2 | 43:RX:89:ILE:HD12 | 1.61 | 0.65 |
| 7:XG:84:ASN:ND2 | 22:XW:34:U:OP1 | 2.26 | 0.65 |
| 1:QA:1245:A:OP2 | 21:QU:9:ARG:NH2 | 2.28 | 0.65 |
| 25:RA:195:A:H61 | 25:RA:198:C:H3' | 1.62 | 0.65 |
| 25:RA:2030:A:H4' | 25:RA:2031:A:H8 | 1.61 | 0.65 |
| 25:RA:2729:G:H1' | 28:RE:187:ALA:HB2 | 1.77 | 0.65 |
| 36:YQ:65:PHE:HB2 | 36:YQ:105:GLU:HB3 | 1.77 | 0.65 |
| 45:YZ:128:VAL:HG22 | 45:YZ:129:SER:H | 1.61 | 0.65 |
| 1:QA:1355:G:H2' | 1:QA:1356:G:C8 | 2.32 | 0.65 |
| 34:RO:68:GLU:HG3 | 34:RO:78:ARG:HD3 | 1.77 | 0.65 |
| 27:YD:35:LYS:NZ | 27:YD:64:ILE:O | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:QB:109:SER:O | 2:QB:113:HIS:ND1 | 2.30 | 0.65 |
| 55:Y9:4:ARG:HB2 | 55:Y9:34:GLN:HB3 | 1.78 | 0.65 |
| 25:YA:2747:G:N1 | 25:YA:2755:C:OP2 | 2.29 | 0.65 |
| 27:RD:168:ARG:HG2 | 27:RD:173:VAL:HG12 | 1.79 | 0.65 |
| 8:XH:10:LEU:HD22 | 8:XH:83:ILE:HD11 | 1.78 | 0.65 |
| 52:Y6:10:LEU:HG | 52:Y6:54:ILE:HD12 | 1.79 | 0.65 |
| 25:YA:24:G:O2' | 42:YW:78:GLU:O | 2.15 | 0.65 |
| 1:QA:1225:A:H4' | 19:QS:78:ARG:HE | 1.62 | 0.64 |
| 25:RA:2466:C:OP1 | 55:R9:22:ARG:NH1 | 2.29 | 0.64 |
| 25:RA:2572:A:H2' | 28:RE:144:ARG:HD3 | 1.78 | 0.64 |
| 25:RA:2731:G:OP1 | 28:RE:169:ASN:ND2 | 2.27 | 0.64 |
| 27:RD:123:ALA:HB3 | 27:RD:131:LEU:HG | 1.79 | 0.64 |
| 25:YA:2744:G:OP2 | 55:Y9:19:ARG:N | 2.30 | 0.64 |
| 25:YA:586:A:H4' | 29:YF:89:VAL:HG11 | 1.79 | 0.64 |
| 1:QA:684:A:O2' | 11:QK:39:PRO:O | 2.14 | 0.64 |
| 1:QA:1073:U:O2 | 2:QB:104:ASN:ND2 | 2.29 | 0.64 |
| 37:RR:103:ARG:NH1 | 42:RW:40:ASN:OD1 | 2.28 | 0.64 |
| 25:YA:1084:A:N1 | 25:YA:1085:A:N6 | 2.45 | 0.64 |
| 31:YH:150:ALA:HA | 55:Y9:19:ARG:HB3 | 1.78 | 0.64 |
| 1:QA:1355:G:H2' | 1:QA:1356:G:H8 | 1.62 | 0.64 |
| 18:QR:74:ARG:HG2 | 18:QR:81:PHE:CE1 | 2.32 | 0.64 |
| 25:RA:270(T):G:H5'' | 47:R1:97:LEU:HD22 | 1.79 | 0.64 |
| 40:RU:85:LYS:NZ | 40:RU:117:GLN:OE1 | 2.29 | 0.64 |
| 25:YA:819:A:OP2 | 25:YA:1187:G:N2 | 2.30 | 0.64 |
| 25:RA:2347:C:OP1 | 52:R6:38:LYS:NZ | 2.27 | 0.64 |
| 2:XB:32:ILE:HD11 | 2:XB:40:HIS:HB3 | 1.78 | 0.64 |
| 4:XD:62:GLN:HE22 | 4:XD:65:ARG:HH21 | 1.45 | 0.64 |
| 25:YA:848:G:H2' | 25:YA:849:A:H8 | 1.61 | 0.64 |
| 7:QG:86:GLN:NE2 | 22:QW:33:C:O2' | 2.30 | 0.64 |
| 11:QK:54:ARG:HH12 | 22:QW:40:C:H4' | 1.61 | 0.64 |
| 30:RG:107:LEU:HD23 | 30:RG:111:LEU:HD12 | 1.78 | 0.64 |
| 1:XA:31:G:HO2' | 1:XA:48:C:N4 | 1.96 | 0.64 |
| 25:YA:589:C:H2' | 25:YA:590:A:C8 | 2.31 | 0.64 |
| 1:QA:297:G:N2 | 1:QA:300:A:OP2 | 2.27 | 0.64 |
| 3:QC:157:ILE:HD13 | 3:QC:166:GLU:HG2 | 1.79 | 0.64 |
| 5:QE:81:GLU:HG2 | 5:QE:90:VAL:HG22 | 1.79 | 0.64 |
| 25:RA:1405:U:H2' | 25:RA:1406:U:H6 | 1.62 | 0.64 |
| 25:RA:1426:G:OP2 | 25:RA:1427:A:O2' | 2.15 | 0.64 |
| 25:RA:675:A:N3 | 25:RA:2443:C:O2' | 2.30 | 0.64 |
| 36:RQ:66:ILE:HA | 36:RQ:104:PHE:HA | 1.80 | 0.64 |
| 38:RS:26:LEU:HB3 | 38:RS:87:PHE:HA | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:134:A:H61 | 16:XP:25:ARG:HH12 | 1.46 | 0.64 |
| 22:QW:59:A:O2' | 22:QW:60:A:OP1 | 2.15 | 0.64 |
| 35:RP:62:LEU:HD23 | 35:RP:62:LEU:H | 1.62 | 0.64 |
| 43:RX:54:VAL:HG22 | 43:RX:81:VAL:HG23 | 1.79 | 0.64 |
| 27:YD:35:LYS:HB3 | 27:YD:36:PRO:CD | 2.25 | 0.64 |
| 31:YH:154:PRO:HG3 | 55:Y9:18:ARG:O | 1.97 | 0.64 |
| 19:QS:10:PHE:HE2 | 19:QS:16:LEU:HB2 | 1.63 | 0.64 |
| 13:XM:3:ARG:HA | 13:XM:9:ILE:HG21 | 1.78 | 0.64 |
| 25:YA:20:C:O2 | 25:YA:520:G:N2 | 2.20 | 0.64 |
| 25:YA:2743:C:C6 | 55:Y9:26:ILE:HG23 | 2.33 | 0.64 |
| 30:YG:16:ARG:NH2 | 30:YG:28:VAL:O | 2.31 | 0.64 |
| 1:QA:429:U:OP2 | 4:QD:36:ARG:NH2 | 2.30 | 0.64 |
| 25:RA:630:G:N2 | 25:RA:633:A:OP2 | 2.31 | 0.64 |
| 17:XQ:6:LEU:HD13 | 17:XQ:23:VAL:HG11 | 1.80 | 0.64 |
| 25:YA:566:U:H5' | 35:YP:29:LYS:HD2 | 1.80 | 0.64 |
| 1:QA:689:C:OP1 | 11:QK:27:ASN:ND2 | 2.31 | 0.64 |
| 8:QH:10:LEU:HD22 | 8:QH:83:ILE:HD11 | 1.78 | 0.64 |
| 33:RN:6:PRO:HG3 | 33:RN:41:ASP:HB2 | 1.80 | 0.64 |
| 1:XA:1432:G:O2' | 1:XA:1468:A:N6 | 2.31 | 0.64 |
| 1:QA:954:G:O6 | 13:QM:104:ARG:NH1 | 2.30 | 0.63 |
| 25:RA:768:G:O2' | 25:RA:1379:A:N6 | 2.29 | 0.63 |
| 1:XA:686:U:H1' | 11:XK:42:TRP:HE1 | 1.62 | 0.63 |
| 50:Y4:16:CYS:SG | 50:Y4:17:GLY:N | 2.71 | 0.63 |
| 1:QA:606:G:H22 | 1:QA:631:G:H5' | 1.62 | 0.63 |
| 1:QA:715:A:H2' | 1:QA:716:A:C8 | 2.33 | 0.63 |
| 22:XV:44:A:H2' | 22:XV:45:A:C8 | 2.33 | 0.63 |
| 25:YA:1042:G:H1 | 25:YA:1113:U:H3 | 1.45 | 0.63 |
| 27:YD:148:GLU:HB2 | 27:YD:151:LYS:HD2 | 1.80 | 0.63 |
| 3:QC:108:ASN:HD21 | 3:QC:144:SER:HB2 | 1.63 | 0.63 |
| 10:QJ:45:ARG:HB3 | 10:QJ:65:LEU:HB3 | 1.80 | 0.63 |
| 25:RA:676:A:H8 | 25:RA:2069:G:H21 | 1.46 | 0.63 |
| 25:YA:2743:C:C5' | 55:Y9:26:ILE:H | 2.11 | 0.63 |
| 25:RA:259:G:H21 | 25:RA:621:A:H8 | 1.47 | 0.63 |
| 1:XA:1175:G:H2' | 1:XA:1176:A:C8 | 2.33 | 0.63 |
| 3:XC:172:ARG:HG2 | 3:XC:174:PRO:HD3 | 1.80 | 0.63 |
| 25:YA:2680:C:H5' | 28:YE:189:PRO:HA | 1.79 | 0.63 |
| 1:QA:624:C:H2' | 1:QA:625:G:H8 | 1.64 | 0.63 |
| 1:XA:191(A):G:H2' | 1:XA:191(B):G:C8 | 2.34 | 0.63 |
| 25:YA:300:A:OP1 | 44:YY:86:ARG:NH2 | 2.32 | 0.63 |
| 1:QA:1160:G:H1 | 1:QA:1177:G:H22 | 1.44 | 0.63 |
| 2:QB:32:ILE:HD11 | 2:QB:40:HIS:HB3 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 10:QJ:42:THR:HG21 | 10:QJ:66:ARG:HG3 | 1.79 | 0.63 |
| 25:RA:1021:A:H61 | 25:RA:1142(A):A:H61 | 1.47 | 0.63 |
| 25:RA:1857:G:H21 | 25:RA:1886:C:N4 | 1.97 | 0.63 |
| 36:YQ:29:PHE:N | 36:YQ:105:GLU:OE2 | 2.28 | 0.63 |
| 1:QA:563:A:H2' | 1:QA:567:G:C8 | 2.34 | 0.63 |
| 25:RA:2354:G:H4' | 46:R0:35:ASN:HD22 | 1.62 | 0.63 |
| 37:RR:51:LEU:HD22 | 37:RR:66:VAL:HG13 | 1.80 | 0.63 |
| 1:XA:578:C:O2' | 1:XA:728:A:N3 | 2.26 | 0.63 |
| 28:RE:24:THR:HG21 | 28:RE:188:VAL:HG11 | 1.79 | 0.63 |
| 41:RV:28:GLU:HB3 | 41:RV:31:ALA:HB2 | 1.80 | 0.63 |
| 1:XA:1003:G:H21 | 1:XA:1005:A:H5' | 1.62 | 0.63 |
| 1:XA:390:C:H2' | 1:XA:391:G:C8 | 2.34 | 0.63 |
| 19:QS:40:ILE:O | 19:QS:41:VAL:HG13 | 1.99 | 0.63 |
| 1:XA:559:A:OP1 | 5:XE:126:ARG:NH2 | 2.29 | 0.63 |
| 6:XF:9:VAL:HB | 6:XF:87:ARG:HB2 | 1.80 | 0.63 |
| 25:YA:998:C:OP2 | 40:YU:58:ARG:NH1 | 2.32 | 0.63 |
| 25:YA:674:G:H1' | 29:YF:74:ARG:HD3 | 1.80 | 0.63 |
| 1:QA:1224:G:O2' | 1:QA:1322:C:OP2 | 2.15 | 0.62 |
| 50:R4:14:ILE:HB | 50:R4:22:ILE:HB | 1.79 | 0.62 |
| 25:RA:1033:U:OP1 | 55:R9:19:ARG:NE | 2.32 | 0.62 |
| 25:RA:1309:G:HO2' | 25:RA:1611:C:HO2' | 1.46 | 0.62 |
| 25:RA:2376:A:H61 | 38:RS:89:ARG:HD3 | 1.64 | 0.62 |
| 25:RA:1329:U:H5'' | 25:RA:1330:C:H5 | 1.64 | 0.62 |
| 25:RA:673:C:OP1 | 29:RF:54:ARG:NH1 | 2.31 | 0.62 |
| 31:RH:89:ILE:HG22 | 31:RH:162:ILE:HG12 | 1.81 | 0.62 |
| 1:XA:1479:C:H2' | 1:XA:1480:G:H8 | 1.64 | 0.62 |
| 31:YH:146:ALA:HA | 55:Y9:20:HIS:O | 1.98 | 0.62 |
| 25:YA:1061:U:H3' | 25:YA:1062:G:H5'' | 1.80 | 0.62 |
| 1:QA:745:C:H2' | 1:QA:746:A:H8 | 1.63 | 0.62 |
| 1:XA:1329:A:N7 | 21:XU:7:ARG:NH2 | 2.47 | 0.62 |
| 25:YA:2743:C:H3' | 55:Y9:24:TYR:C | 2.19 | 0.62 |
| 25:YA:2743:C:C2 | 55:Y9:26:ILE:HG12 | 2.34 | 0.62 |
| 25:YA:2616:C:H2' | 25:YA:2617:C:H6 | 1.63 | 0.62 |
| 25:RA:2867:G:OP2 | 39:RT:119:LYS:NZ | 2.25 | 0.62 |
| 29:RF:143:ALA:HB1 | 29:RF:148:LEU:HB2 | 1.82 | 0.62 |
| 1:XA:1266:G:N2 | 1:XA:1269:A:OP2 | 2.29 | 0.62 |
| 1:XA:877:C:H2' | 1:XA:878:G:H8 | 1.64 | 0.62 |
| 7:XG:15:ASP:HB3 | 7:XG:19:GLY:H | 1.63 | 0.62 |
| 25:YA:1607:C:N4 | 25:YA:1622:G:OP2 | 2.25 | 0.62 |
| 25:YA:1930:G:N2 | 25:YA:1969:A:OP2 | 2.25 | 0.62 |
| 25:YA:1678:G:N2 | 25:YA:1989:G:H22 | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:48:PHE:HA | 45:YZ:51:ALA:HB3 | 1.81 | 0.62 |
| 25:RA:144:C:H2' | 25:RA:145:G:H8 | 1.64 | 0.62 |
| 40:RU:90:VAL:HG22 | 41:RV:39:LEU:HD23 | 1.82 | 0.62 |
| 45:RZ:102:LEU:HD11 | 45:RZ:124:ILE:HG13 | 1.80 | 0.62 |
| 8:XH:112:LEU:HD23 | 8:XH:133:LEU:HA | 1.81 | 0.62 |
| 25:YA:879:G:N1 | 25:YA:898:C:N3 | 2.34 | 0.62 |
| 27:YD:123:ALA:HB3 | 27:YD:131:LEU:HG | 1.82 | 0.62 |
| 45:YZ:13:GLU:HB3 | 45:YZ:18:LEU:HD11 | 1.82 | 0.62 |
| 1:QA:1119:C:H2' | 1:QA:1120:G:H8 | 1.65 | 0.62 |
| 35:RP:61:ARG:HG3 | 54:R8:13:ARG:HD3 | 1.81 | 0.62 |
| 25:RA:1668:A:N3 | 25:RA:1670:C:N4 | 2.48 | 0.62 |
| 25:RA:589:C:H2' | 25:RA:590:A:H8 | 1.65 | 0.62 |
| 38:YS:20:ARG:NH2 | 46:Y0:51:VAL:O | 2.33 | 0.62 |
| 13:QM:99:ARG:HB2 | 13:QM:101:GLN:HE22 | 1.64 | 0.62 |
| 25:RA:1607:C:N4 | 25:RA:1622:G:OP2 | 2.32 | 0.62 |
| 25:RA:1693:U:O2 | 27:RD:14:ARG:NH1 | 2.33 | 0.62 |
| 25:RA:946:G:O6 | 25:RA:972:G:N2 | 2.33 | 0.62 |
| 25:RA:2086:U:H2' | 25:RA:2087:G:C8 | 2.34 | 0.62 |
| 22:XW:59:A:O2' | 22:XW:60:A:OP1 | 2.15 | 0.62 |
| 29:YF:63:LYS:NZ | 29:YF:75:HIS:O | 2.30 | 0.62 |
| 1:XA:191:G:O2' | 20:XT:101:GLY:O | 2.18 | 0.62 |
| 25:YA:2742:C:O4' | 55:Y9:29:ASN:O | 2.17 | 0.62 |
| 22:QW:34:U:H3' | 22:QW:35:C:H5'' | 1.81 | 0.62 |
| 30:RG:3:LEU:HD11 | 50:R4:25:TYR:CE2 | 2.35 | 0.62 |
| 25:RA:1518:C:H2' | 25:RA:1519:G:H8 | 1.63 | 0.62 |
| 28:RE:52:LEU:O | 28:RE:74:PRO:HA | 1.99 | 0.62 |
| 25:YA:2539:C:H1' | 55:Y9:29:ASN:HD21 | 1.65 | 0.62 |
| 9:QI:63:ILE:HG21 | 9:QI:77:ILE:HG12 | 1.81 | 0.61 |
| 1:QA:1061:G:OP1 | 10:QJ:59:SER:OG | 2.18 | 0.61 |
| 1:XA:738:C:H5'' | 6:XF:69:GLU:HB2 | 1.82 | 0.61 |
| 1:XA:675:A:H1' | 11:XK:116:HIS:CD2 | 2.33 | 0.61 |
| 25:YA:2438:U:O3' | 25:YA:2439:A:H3' | 2.00 | 0.61 |
| 40:YU:90:VAL:HG22 | 41:YV:39:LEU:HD23 | 1.82 | 0.61 |
| 25:RA:184:C:O2' | 25:RA:217:G:N3 | 2.32 | 0.61 |
| 25:RA:2503:A:O2' | 25:RA:2505:G:OP2 | 2.16 | 0.61 |
| 27:RD:148:GLU:HB2 | 27:RD:151:LYS:HD2 | 1.81 | 0.61 |
| 37:RR:55:ALA:HA | 37:RR:80:PHE:CE1 | 2.35 | 0.61 |
| 25:YA:2742:C:O2' | 55:Y9:25:VAL:O | 2.18 | 0.61 |
| 25:YA:1980:G:O2' | 25:YA:1982:C:OP2 | 2.15 | 0.61 |
| 25:YA:221:A:H4' | 25:YA:222:A:O5' | 2.00 | 0.61 |
| 25:YA:2737:G:H2' | 25:YA:2738:A:C8 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:YD:94:LEU:HD13 | 27:YD:104:TYR:HE1 | 1.65 | 0.61 |
| 1:QA:346:G:H1' | 1:QA:347:G:H5' | 1.82 | 0.61 |
| 1:XA:1287:A:H2 | 1:XA:1353:G:H1' | 1.65 | 0.61 |
| 25:YA:2514:U:H2' | 25:YA:2515:C:H6 | 1.64 | 0.61 |
| 25:YA:460:A:N6 | 25:YA:469:G:H21 | 1.97 | 0.61 |
| 47:R1:18:ILE:HG12 | 47:R1:37:ILE:HG12 | 1.81 | 0.61 |
| 25:RA:1206:G:H1 | 25:RA:1240:U:H3 | 1.49 | 0.61 |
| 2:XB:5:ILE:HB | 2:XB:221:LEU:HD23 | 1.81 | 0.61 |
| 5:XE:34:VAL:HG11 | 5:XE:63:ARG:HE | 1.64 | 0.61 |
| 55:Y9:24:TYR:O | 55:Y9:25:VAL:HG13 | 2.01 | 0.61 |
| 25:YA:2314:C:H2' | 25:YA:2315:G:H8 | 1.64 | 0.61 |
| 1:QA:26:A:O2' | 4:QD:209:ARG:NH2 | 2.31 | 0.61 |
| 25:RA:2527:C:OP1 | 55:R9:2:LYS:NZ | 2.31 | 0.61 |
| 28:RE:76:ARG:HD3 | 28:RE:195:LEU:HD22 | 1.83 | 0.61 |
| 18:XR:74:ARG:HG2 | 18:XR:81:PHE:CE1 | 2.35 | 0.61 |
| 25:YA:2473:U:OP1 | 25:YA:2529:G:N2 | 2.33 | 0.61 |
| 25:YA:2743:C:H3' | 55:Y9:25:VAL:HA | 1.83 | 0.61 |
| 28:YE:52:LEU:O | 28:YE:74:PRO:HA | 2.00 | 0.61 |
| 31:YH:142:GLY:O | 31:YH:146:ALA:HB2 | 2.00 | 0.61 |
| 31:YH:10:PRO:HG3 | 31:YH:69:ARG:HH12 | 1.66 | 0.61 |
| 1:QA:1510:U:H2' | 1:QA:1511:G:C8 | 2.36 | 0.61 |
| 19:QS:50:ALA:HB1 | 19:QS:57:HIS:HB3 | 1.82 | 0.61 |
| 25:RA:1105:U:H2' | 25:RA:1106:G:H8 | 1.65 | 0.61 |
| 25:RA:1678:G:H22 | 25:RA:1989:G:N2 | 1.98 | 0.61 |
| 29:RF:32:LEU:HD11 | 29:RF:105:VAL:HG13 | 1.82 | 0.61 |
| 45:RZ:145:GLU:HG3 | 45:RZ:146:ILE:H | 1.65 | 0.61 |
| 55:Y9:24:TYR:CZ | 55:Y9:35:ARG:HG3 | 2.35 | 0.61 |
| 26:YB:33:G:OP2 | 30:YG:96:ARG:NH2 | 2.32 | 0.61 |
| 27:YD:17:THR:O | 27:YD:211:ARG:NH1 | 2.33 | 0.61 |
| 29:YF:182:ASN:O | 29:YF:186:ILE:HG12 | 2.01 | 0.61 |
| 12:QL:53:ARG:HH12 | 12:QL:92:ASP:HB2 | 1.66 | 0.61 |
| 25:RA:746:A:O2' | 25:RA:2611:U:O2' | 2.19 | 0.61 |
| 17:XQ:66:SER:O | 17:XQ:70:ARG:NH1 | 2.33 | 0.61 |
| 25:YA:2327:A:H2' | 25:YA:2328:A:C8 | 2.35 | 0.61 |
| 27:YD:31:LYS:HG3 | 27:YD:32:SER:H | 1.64 | 0.61 |
| 25:RA:2747:G:H21 | 25:RA:2757:A:H62 | 0.71 | 0.61 |
| 25:RA:372:G:N2 | 25:RA:401:A:OP2 | 2.33 | 0.61 |
| 29:RF:182:ASN:O | 29:RF:186:ILE:HG12 | 2.00 | 0.61 |
| 36:RQ:43:THR:HG22 | 36:RQ:94:VAL:HG12 | 1.81 | 0.61 |
| 1:XA:1513:A:H2' | 1:XA:1514:C:C6 | 2.36 | 0.61 |
| 28:YE:78:LEU:HG | 28:YE:79:ARG:HG2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:YI:30:LEU:HB3 | 32:YI:36:ALA:HB3 | 1.81 | 0.61 |
| 45:YZ:30:ASN:OD1 | 45:YZ:33:LEU:N | 2.31 | 0.61 |
| 10:QJ:3:LYS:N | 10:QJ:74:ILE:O | 2.34 | 0.61 |
| 1:QA:134:A:N6 | 16:QP:25:ARG:HH12 | 1.99 | 0.61 |
| 25:RA:2469:A:H5'' | 25:RA:2470:G:C8 | 2.35 | 0.61 |
| 25:RA:321:G:O2' | 25:RA:340:A:N3 | 2.34 | 0.61 |
| 1:XA:1291:G:O2' | 9:XI:38:GLN:OE1 | 2.19 | 0.61 |
| 3:XC:70:VAL:HG12 | 3:XC:72:LYS:H | 1.66 | 0.61 |
| 4:XD:19:LEU:HD13 | 4:XD:67:ILE:HA | 1.82 | 0.61 |
| 25:YA:679:C:H2' | 25:YA:680:G:H8 | 1.66 | 0.61 |
| 29:YF:117:ARG:HH21 | 29:YF:187:VAL:HA | 1.66 | 0.61 |
| 30:YG:80:PHE:HE2 | 30:YG:82:LEU:HD12 | 1.66 | 0.61 |
| 40:YU:91:ASP:O | 40:YU:95:LEU:N | 2.33 | 0.61 |
| 11:QK:86:GLY:O | 11:QK:91:ARG:NH1 | 2.34 | 0.61 |
| 1:QA:1309:G:N7 | 13:QM:99:ARG:NH2 | 2.48 | 0.61 |
| 1:XA:264:U:O2' | 17:XQ:64:PRO:O | 2.17 | 0.61 |
| 25:YA:2526:G:C1' | 55:Y9:28:GLU:HB3 | 2.31 | 0.61 |
| 25:YA:813:U:H2' | 25:YA:814:C:C6 | 2.36 | 0.61 |
| 31:YH:28:GLY:HA3 | 31:YH:79:VAL:HB | 1.81 | 0.61 |
| 1:QA:1367:C:H4' | 10:QJ:48:THR:HG21 | 1.83 | 0.60 |
| 6:QF:9:VAL:HB | 6:QF:87:ARG:HB2 | 1.82 | 0.60 |
| 10:QJ:38:ILE:HD11 | 10:QJ:71:LEU:HD23 | 1.83 | 0.60 |
| 25:RA:1754:C:OP1 | 39:RT:96:ARG:NH1 | 2.34 | 0.60 |
| 25:RA:2438:U:O3' | 25:RA:2439:A:H3' | 2.01 | 0.60 |
| 25:RA:764:A:H5' | 27:RD:210:GLY:HA2 | 1.83 | 0.60 |
| 37:RR:24:GLN:HG3 | 37:RR:44:LEU:HD13 | 1.83 | 0.60 |
| 1:XA:407:G:H2' | 1:XA:408:A:H8 | 1.66 | 0.60 |
| 1:XA:80:G:O6 | 1:XA:89:U:O4 | 2.18 | 0.60 |
| 13:XM:99:ARG:HB2 | 13:XM:101:GLN:HE22 | 1.65 | 0.60 |
| 26:YB:43:C:H4' | 30:YG:98:ARG:HH22 | 1.66 | 0.60 |
| 3:QC:95:THR:HG22 | 3:QC:97:LYS:H | 1.66 | 0.60 |
| 17:QQ:66:SER:O | 17:QQ:70:ARG:NH1 | 2.33 | 0.60 |
| 22:QW:15:G:H2' | 22:QW:60:A:N1 | 2.16 | 0.60 |
| 25:RA:665:C:H2' | 25:RA:666:G:H8 | 1.65 | 0.60 |
| 25:RA:749:C:H5' | 25:RA:1271:G:H1' | 1.83 | 0.60 |
| 27:RD:17:THR:O | 27:RD:211:ARG:NH1 | 2.34 | 0.60 |
| 1:XA:745:C:H2' | 1:XA:746:A:H8 | 1.65 | 0.60 |
| 47:Y1:17:SER:HB2 | 47:Y1:40:ARG:HD2 | 1.83 | 0.60 |
| 27:YD:43:ARG:HH11 | 27:YD:49:ILE:HD12 | 1.66 | 0.60 |
| 30:YG:125:PHE:HE2 | 30:YG:170:ARG:HB2 | 1.64 | 0.60 |
| 37:YR:17:ARG:HG2 | 37:YR:21:TYR:CE2 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:20:U:O2' | 1:QA:573:A:N6 | 2.35 | 0.60 |
| 1:QA:985:C:H2' | 1:QA:986:A:H8 | 1.65 | 0.60 |
| 25:RA:2296:U:OP2 | 38:RS:9:ARG:NH1 | 2.35 | 0.60 |
| 4:XD:98:GLU:HG2 | 4:XD:189:PRO:HG3 | 1.83 | 0.60 |
| 1:XA:1291:G:H5'' | 7:XG:41:ARG:HH21 | 1.66 | 0.60 |
| 25:YA:299:A:N1 | 25:YA:322:A:O2' | 2.27 | 0.60 |
| 35:YP:101:VAL:HB | 35:YP:106:LEU:HB2 | 1.82 | 0.60 |
| 28:YE:10:GLY:HA3 | 39:YT:8:LYS:HD3 | 1.83 | 0.60 |
| 25:RA:1348:G:H2' | 25:RA:1349:A:H5'' | 1.83 | 0.60 |
| 6:XF:68:PRO:HG3 | 6:XF:71:ARG:HH21 | 1.65 | 0.60 |
| 13:XM:14:ARG:HH12 | 13:XM:42:ALA:HA | 1.66 | 0.60 |
| 25:YA:1430:C:H2' | 25:YA:1431:U:C6 | 2.37 | 0.60 |
| 25:YA:259:G:H21 | 25:YA:621:A:H8 | 1.48 | 0.60 |
| 25:YA:918:A:N3 | 26:YB:80:U:O2' | 2.34 | 0.60 |
| 1:QA:1314:C:H2' | 1:QA:1315:U:H6 | 1.67 | 0.60 |
| 25:RA:1011:G:H1 | 25:RA:1150:C:H42 | 1.47 | 0.60 |
| 25:RA:514:A:N3 | 25:RA:581:C:O2' | 2.33 | 0.60 |
| 1:XA:477:G:H2' | 1:XA:478:A:H8 | 1.66 | 0.60 |
| 28:YE:201:THR:HG22 | 28:YE:203:LYS:H | 1.64 | 0.60 |
| 33:YN:99:LEU:HD12 | 33:YN:122:VAL:HG21 | 1.82 | 0.60 |
| 2:QB:115:LEU:HD13 | 2:QB:145:LEU:HB3 | 1.83 | 0.60 |
| 4:QD:19:LEU:HD12 | 4:QD:21:LEU:HG | 1.83 | 0.60 |
| 25:RA:674:G:H1' | 29:RF:74:ARG:HD3 | 1.81 | 0.60 |
| 42:RW:86:LEU:HD22 | 42:RW:96:ILE:HD11 | 1.83 | 0.60 |
| 1:XA:439:A:OP2 | 1:XA:493:G:N1 | 2.34 | 0.60 |
| 13:XM:14:ARG:NH2 | 13:XM:16:ASP:OD2 | 2.34 | 0.60 |
| 25:YA:2746:U:OP2 | 55:Y9:35:ARG:NH2 | 2.35 | 0.60 |
| 25:RA:2010:G:H5'' | 42:RW:42:ARG:HB2 | 1.82 | 0.60 |
| 27:RD:85:ASP:OD2 | 27:RD:88:ARG:NH1 | 2.31 | 0.60 |
| 1:XA:346:G:O2' | 1:XA:347:G:O4' | 2.17 | 0.60 |
| 25:YA:1728:G:N1 | 25:YA:1730:U:OP2 | 2.34 | 0.60 |
| 25:YA:2126:A:H4' | 25:YA:2127:G:O5' | 2.01 | 0.60 |
| 1:QA:712:A:H2' | 1:QA:713:G:C8 | 2.37 | 0.60 |
| 7:QG:116:ALA:HA | 7:QG:119:ARG:HE | 1.66 | 0.60 |
| 10:QJ:39:PRO:HB3 | 10:QJ:70:ARG:NH1 | 2.17 | 0.60 |
| 13:QM:3:ARG:HA | 13:QM:9:ILE:HG21 | 1.84 | 0.60 |
| 25:RA:1363:C:O2' | 25:RA:1809:A:N3 | 2.31 | 0.60 |
| 1:XA:514:C:H2' | 1:XA:515:G:H8 | 1.67 | 0.60 |
| 35:YP:50:ARG:HB2 | 54:Y8:59:LYS:HD3 | 1.84 | 0.60 |
| 25:YA:1195:G:O6 | 35:YP:16:ARG:NH2 | 2.32 | 0.60 |
| 25:YA:574:C:N3 | 28:YE:145:LYS:NZ | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:55:ASN:ND2 | 28:YE:75:VAL:HG22 | 2.17 | 0.60 |
| 29:YF:31:HIS:NE2 | 29:YF:35:GLU:OE2 | 2.34 | 0.60 |
| 25:RA:2021:C:OP1 | 51:R5:12:SER:OG | 2.13 | 0.60 |
| 45:RZ:48:PHE:HA | 45:RZ:51:ALA:HB3 | 1.83 | 0.60 |
| 25:RA:1636:C:H2' | 25:RA:1637:A:C8 | 2.37 | 0.60 |
| 14:YN:21:TYR:OH | 14:YN:23:ARG:NH2 | 2.32 | 0.60 |
| 46:Y0:23:VAL:HG13 | 46:Y0:38:VAL:HG22 | 1.83 | 0.60 |
| 25:YA:1348:G:H2' | 25:YA:1349:A:H5'' | 1.83 | 0.60 |
| 25:YA:890:A:H2' | 25:YA:892:G:H8 | 1.67 | 0.60 |
| 1:QA:339:C:OP2 | 34:RO:97:ARG:NH1 | 2.35 | 0.59 |
| 15:QO:39:LEU:HD11 | 15:QO:52:SER:HB3 | 1.84 | 0.59 |
| 25:RA:2561:A:H4' | 34:RO:40:VAL:HG11 | 1.84 | 0.59 |
| 1:XA:1151:A:O2' | 10:XJ:70:ARG:NH2 | 2.35 | 0.59 |
| 1:XA:34:C:H2' | 1:XA:35:G:H8 | 1.67 | 0.59 |
| 11:XK:34:ASP:OD1 | 11:XK:38:ASN:N | 2.35 | 0.59 |
| 45:YZ:163:LEU:HD22 | 45:YZ:167:PRO:HG3 | 1.84 | 0.59 |
| 25:RA:288:C:H2' | 25:RA:289:A:H8 | 1.67 | 0.59 |
| 28:RE:114:ALA:HB3 | 28:RE:160:TYR:HB3 | 1.84 | 0.59 |
| 35:RP:106:LEU:HD21 | 35:RP:112:LEU:HD13 | 1.84 | 0.59 |
| 44:RY:52:SER:HB2 | 44:RY:53:PRO:HD2 | 1.84 | 0.59 |
| 1:XA:674:G:O6 | 1:XA:716:A:N1 | 2.34 | 0.59 |
| 14:YN:29:ARG:HD3 | 14:YN:40:CYS:HB2 | 1.84 | 0.59 |
| 18:XR:32:ARG:HA | 18:XR:69:THR:HG21 | 1.83 | 0.59 |
| 25:YA:2514:U:H2' | 25:YA:2515:C:C6 | 2.37 | 0.59 |
| 35:YP:62:LEU:H | 35:YP:62:LEU:HD23 | 1.66 | 0.59 |
| 1:QA:1433:A:OP2 | 1:QA:1467:G:N1 | 2.33 | 0.59 |
| 1:QA:562:C:H1' | 12:QL:15:ARG:HD2 | 1.83 | 0.59 |
| 13:QM:57:ARG:O | 13:QM:61:GLU:HG2 | 2.02 | 0.59 |
| 22:QV:44:A:H2' | 22:QV:45:A:C8 | 2.37 | 0.59 |
| 53:R7:10:ARG:HE | 53:R7:14:LYS:HD2 | 1.67 | 0.59 |
| 25:RA:1853:A:N3 | 25:RA:2233:U:O2' | 2.30 | 0.59 |
| 31:RH:87:LEU:HD22 | 31:RH:149:ARG:HD3 | 1.84 | 0.59 |
| 35:RP:101:VAL:HG21 | 35:RP:108:LYS:HD2 | 1.84 | 0.59 |
| 1:XA:1286:A:H2' | 1:XA:1287:A:H4' | 1.84 | 0.59 |
| 48:Y2:18:PRO:HA | 48:Y2:21:LEU:HD12 | 1.85 | 0.59 |
| 25:YA:2525:G:N2 | 55:Y9:28:GLU:HG3 | 2.12 | 0.59 |
| 25:YA:1359:A:N6 | 25:YA:1372:U:H3 | 2.00 | 0.59 |
| 25:YA:2538:C:H2' | 25:YA:2539:C:C6 | 2.37 | 0.59 |
| 25:YA:848:G:H2' | 25:YA:849:A:C8 | 2.37 | 0.59 |
| 28:YE:131:ALA:O | 28:YE:134:ILE:HG13 | 2.03 | 0.59 |
| 2:QB:68:ILE:HG12 | 2:QB:161:ALA:HB3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:RI:27:ARG:HB2 | 47:R1:71:TYR:HE2 | 1.66 | 0.59 |
| 25:RA:2466:C:H2' | 25:RA:2467:C:C6 | 2.36 | 0.59 |
| 25:RA:274:G:N2 | 25:RA:363:G:O6 | 2.35 | 0.59 |
| 25:RA:566:U:H5'' | 35:RP:29:LYS:HD2 | 1.84 | 0.59 |
| 30:RG:82:LEU:HD21 | 30:RG:88:ILE:HG12 | 1.84 | 0.59 |
| 25:YA:2291:U:H2' | 25:YA:2292:C:C6 | 2.37 | 0.59 |
| 25:YA:993:G:OP1 | 40:YU:50:ARG:NH2 | 2.30 | 0.59 |
| 39:YT:51:ARG:HG2 | 39:YT:98:LYS:HE3 | 1.82 | 0.59 |
| 1:QA:708:C:OP1 | 11:QK:85:ARG:NH2 | 2.28 | 0.59 |
| 2:QB:47:THR:HA | 2:QB:202:PRO:HG2 | 1.85 | 0.59 |
| 4:QD:19:LEU:HD13 | 4:QD:67:ILE:HA | 1.83 | 0.59 |
| 25:RA:2111:C:N3 | 25:RA:2118:U:O2' | 2.33 | 0.59 |
| 25:RA:84:A:N7 | 25:RA:99:U:N3 | 2.50 | 0.59 |
| 25:YA:618:G:H5' | 29:YF:205:ARG:HH21 | 1.66 | 0.59 |
| 25:YA:864:G:H1' | 25:YA:914:C:H42 | 1.66 | 0.59 |
| 27:YD:39:LYS:NZ | 27:YD:87:ASN:OD1 | 2.28 | 0.59 |
| 37:YR:86:ARG:NH2 | 37:YR:118:GLU:OXT | 2.36 | 0.59 |
| 1:QA:806:C:H2' | 1:QA:807:A:C8 | 2.37 | 0.59 |
| 2:QB:67:THR:HG21 | 2:QB:155:LEU:HD11 | 1.85 | 0.59 |
| 25:RA:883:G:H22 | 25:RA:892:G:H22 | 1.51 | 0.59 |
| 30:RG:145:THR:OG1 | 30:RG:147:ASP:OD1 | 2.18 | 0.59 |
| 31:RH:8:PRO:HG2 | 31:RH:69:ARG:NE | 2.14 | 0.59 |
| 4:XD:10:ARG:HG3 | 4:XD:40:PRO:HG3 | 1.83 | 0.59 |
| 22:XW:15:G:H2' | 22:XW:60:A:N1 | 2.17 | 0.59 |
| 26:YB:48:A:OP2 | 38:YS:30:ARG:NH2 | 2.36 | 0.59 |
| 1:QA:235:C:H2' | 1:QA:236:G:H8 | 1.68 | 0.59 |
| 1:QA:851:G:H2' | 1:QA:852:G:C8 | 2.37 | 0.59 |
| 1:QA:827:U:H5 | 1:QA:870:U:C2 | 2.21 | 0.59 |
| 1:XA:157:G:H1 | 1:XA:164:U:H3 | 1.49 | 0.59 |
| 1:XA:452:A:O2' | 16:XP:72:ARG:NH1 | 2.36 | 0.59 |
| 54:Y8:29:LYS:HB2 | 54:Y8:33:ASN:ND2 | 2.18 | 0.59 |
| 25:YA:1141:U:H1' | 25:YA:1142(A):A:C6 | 2.38 | 0.59 |
| 28:YE:114:ALA:HB3 | 28:YE:160:TYR:HB3 | 1.84 | 0.59 |
| 10:QJ:51:ARG:O | 14:QN:45:ARG:NH1 | 2.36 | 0.59 |
| 22:QV:35:C:H2' | 22:QV:36:A:H8 | 1.68 | 0.59 |
| 48:R2:18:PRO:HA | 48:R2:21:LEU:HD12 | 1.85 | 0.59 |
| 53:R7:35:ARG:HE | 53:R7:42:LEU:HD13 | 1.67 | 0.59 |
| 25:RA:1026:U:H4' | 25:RA:1027:A:OP1 | 2.03 | 0.59 |
| 25:RA:2392:A:H2 | 25:RA:2424:C:H42 | 1.50 | 0.59 |
| 25:RA:297:C:OP1 | 44:RY:87:LYS:NZ | 2.32 | 0.59 |
| 25:RA:569:U:O2' | 25:RA:983:A:N1 | 2.31 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1006:C:H5' | 33:RN:28:THR:HG23 | 1.84 | 0.59 |
| 1:XA:1250:A:N3 | 1:XA:1370:G:O2' | 2.32 | 0.59 |
| 25:YA:2746:U:H5 | 55:Y9:35:ARG:HH12 | 1.50 | 0.59 |
| 25:YA:414:C:H2' | 25:YA:415:A:H8 | 1.68 | 0.59 |
| 36:YQ:81:VAL:HG23 | 36:YQ:82:ARG:H | 1.66 | 0.59 |
| 38:YS:15:ARG:HG3 | 38:YS:19:LYS:HE2 | 1.84 | 0.59 |
| 40:YU:92:ARG:C | 40:YU:94:ASN:H | 2.05 | 0.59 |
| 1:XA:1137:C:HO2' | 1:XA:1138:G:N2 | 2.00 | 0.59 |
| 12:XL:70:ILE:HG12 | 12:XL:100:ILE:HD12 | 1.83 | 0.59 |
| 25:YA:1266:G:O5' | 42:YW:15:ARG:NH2 | 2.35 | 0.59 |
| 28:YE:24:THR:HG21 | 28:YE:188:VAL:HG11 | 1.85 | 0.59 |
| 36:YQ:31:ASP:OD1 | 36:YQ:134:ARG:NH1 | 2.36 | 0.59 |
| 1:QA:17:U:H2' | 1:QA:18:C:C6 | 2.38 | 0.59 |
| 25:RA:1399:C:H2' | 25:RA:1400:G:H8 | 1.67 | 0.59 |
| 25:RA:185:U:H5' | 25:RA:217:G:H21 | 1.68 | 0.59 |
| 25:RA:576:U:H2' | 25:RA:577:G:C8 | 2.38 | 0.59 |
| 29:RF:181:LEU:HD11 | 29:RF:186:ILE:HD11 | 1.84 | 0.59 |
| 1:XA:243:A:H4' | 1:XA:244:U:H3' | 1.84 | 0.59 |
| 1:XA:827:U:O2 | 1:XA:874:G:N2 | 2.36 | 0.59 |
| 15:XO:79:ARG:HA | 15:XO:82:ILE:HG12 | 1.85 | 0.59 |
| 47:Y1:90:ILE:HD12 | 47:Y1:94:LEU:HD12 | 1.85 | 0.59 |
| 25:YA:814:C:H1' | 25:YA:1226:G:H21 | 1.68 | 0.59 |
| 25:YA:1316:U:H2' | 25:YA:1317:A:C8 | 2.37 | 0.59 |
| 25:YA:2630:G:H2' | 25:YA:2631:G:H8 | 1.67 | 0.59 |
| 25:YA:345:A:N3 | 25:YA:347:A:N6 | 2.51 | 0.59 |
| 25:YA:911:A:H2' | 36:YQ:9:TYR:HE2 | 1.68 | 0.59 |
| 43:YX:55:ASN:HB2 | 43:YX:80:ILE:HG23 | 1.84 | 0.59 |
| 4:QD:4:TYR:OH | 4:QD:10:ARG:NH2 | 2.36 | 0.58 |
| 22:QW:17:C:OP1 | 22:QW:61:U:O2' | 2.21 | 0.58 |
| 25:RA:2086:U:H2' | 25:RA:2087:G:H8 | 1.68 | 0.58 |
| 25:RA:782:A:O2' | 27:RD:225:ALA:O | 2.19 | 0.58 |
| 30:RG:5:VAL:HG11 | 30:RG:100:TRP:HB3 | 1.85 | 0.58 |
| 40:RU:92:ARG:C | 40:RU:94:ASN:H | 2.06 | 0.58 |
| 25:YA:517:C:OP1 | 51:Y5:16:ARG:NH2 | 2.35 | 0.58 |
| 25:YA:2526:G:H21 | 55:Y9:13:LYS:NZ | 2.01 | 0.58 |
| 25:YA:554:U:H2' | 25:YA:556:G:C8 | 2.38 | 0.58 |
| 25:YA:780:G:H21 | 25:YA:783:A:H62 | 1.51 | 0.58 |
| 25:YA:864:G:H1' | 25:YA:914:C:N4 | 2.17 | 0.58 |
| 29:YF:65:TRP:NE1 | 29:YF:73:ALA:O | 2.29 | 0.58 |
| 30:YG:9:ARG:O | 30:YG:13:GLU:HG2 | 2.02 | 0.58 |
| 1:XA:1002:G:H2' | 1:XA:1003:G:C8 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:414:C:H2' | 25:YA:415:A:C8 | 2.38 | 0.58 |
| 30:YG:65:GLY:HA3 | 50:Y4:9:LEU:HD21 | 1.85 | 0.58 |
| 18:QR:53:ARG:HH21 | 18:QR:59:SER:HA | 1.67 | 0.58 |
| 30:RG:32:PRO:HB3 | 30:RG:163:ALA:HB2 | 1.83 | 0.58 |
| 25:RA:24:G:O2' | 42:RW:78:GLU:O | 2.21 | 0.58 |
| 15:XO:17:ARG:HH12 | 15:XO:77:ARG:HH11 | 1.50 | 0.58 |
| 25:YA:593:G:H4' | 54:Y8:61:LEU:HD13 | 1.84 | 0.58 |
| 25:YA:1270:C:H5'' | 25:YA:1271:G:H5' | 1.84 | 0.58 |
| 43:YX:12:VAL:HB | 43:YX:27:THR:HG23 | 1.85 | 0.58 |
| 2:QB:25:ASN:ND2 | 2:QB:193:ASP:HB3 | 2.18 | 0.58 |
| 4:QD:100:ARG:NH2 | 4:QD:136:PRO:O | 2.37 | 0.58 |
| 25:RA:577:G:O2' | 25:RA:1254:A:OP1 | 2.21 | 0.58 |
| 25:RA:1812:A:H4' | 27:RD:46:GLN:HE22 | 1.67 | 0.58 |
| 25:RA:414:C:O2 | 25:RA:1864:U:O2' | 2.21 | 0.58 |
| 1:XA:1305:G:OP1 | 21:XU:2:GLY:N | 2.36 | 0.58 |
| 25:YA:1819:A:H5'' | 27:YD:161:THR:HG21 | 1.85 | 0.58 |
| 24:XY:37:A:O2' | 25:YA:1913:A:N1 | 2.35 | 0.58 |
| 25:YA:2313:C:H5'' | 30:YG:91:ARG:HD3 | 1.85 | 0.58 |
| 29:YF:63:LYS:HE2 | 29:YF:67:GLN:HB2 | 1.84 | 0.58 |
| 39:YT:50:ILE:HG13 | 39:YT:99:LEU:HD12 | 1.85 | 0.58 |
| 41:YV:28:GLU:HB3 | 41:YV:31:ALA:HB2 | 1.85 | 0.58 |
| 1:QA:1469:G:H2' | 1:QA:1470:G:H8 | 1.69 | 0.58 |
| 1:QA:581:G:OP1 | 15:QO:65:ARG:NH1 | 2.34 | 0.58 |
| 3:QC:150:LYS:HE2 | 3:QC:152:ILE:HD11 | 1.85 | 0.58 |
| 3:QC:172:ARG:HG2 | 3:QC:174:PRO:HD3 | 1.86 | 0.58 |
| 25:RA:1859:A:N6 | 25:RA:1883:G:O2' | 2.36 | 0.58 |
| 25:RA:363(F):A:H1' | 25:RA:364:C:H5 | 1.69 | 0.58 |
| 1:XA:1330:U:H4' | 13:XM:23:TYR:CE1 | 2.39 | 0.58 |
| 4:XD:19:LEU:HD12 | 4:XD:21:LEU:HG | 1.86 | 0.58 |
| 16:XP:3:LYS:HG3 | 16:XP:65:GLN:O | 2.02 | 0.58 |
| 25:YA:587:C:OP2 | 35:YP:21:ARG:NH1 | 2.32 | 0.58 |
| 1:QA:673:G:H2' | 1:QA:674:G:C8 | 2.39 | 0.58 |
| 25:RA:2512:C:O2' | 28:RE:154:LYS:NZ | 2.25 | 0.58 |
| 25:RA:582:G:H2' | 25:RA:583:G:C8 | 2.39 | 0.58 |
| 1:XA:1305:G:N2 | 1:XA:1332:A:OP2 | 2.37 | 0.58 |
| 25:YA:2521:C:O2' | 25:YA:2564:A:N3 | 2.34 | 0.58 |
| 25:YA:2742:C:H1' | 55:Y9:26:ILE:CA | 2.21 | 0.58 |
| 37:YR:55:ALA:HA | 37:YR:80:PHE:CE1 | 2.38 | 0.58 |
| 39:YT:111:ARG:C | 39:YT:113:LYS:H | 2.07 | 0.58 |
| 45:YZ:145:GLU:HG3 | 45:YZ:146:ILE:H | 1.68 | 0.58 |
| 1:QA:1366:C:O2' | 10:QJ:60:ARG:NH1 | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:QW:72:C:HO2' | 25:RA:1851:U:HO2' | 1.50 | 0.58 |
| 25:RA:2752:C:H3' | 25:RA:2753:A:H8 | 1.68 | 0.58 |
| 25:RA:27:G:HO2' | 25:RA:28:A:H8 | 1.51 | 0.58 |
| 42:RW:22:ASP:OD1 | 42:RW:25:ARG:NH1 | 2.34 | 0.58 |
| 8:XH:17:THR:O | 8:XH:78:GLN:NE2 | 2.37 | 0.58 |
| 22:XW:8:U:C2 | 22:XW:14:A:N7 | 2.72 | 0.58 |
| 49:Y3:39:ASP:OD1 | 49:Y3:44:ARG:NH2 | 2.35 | 0.58 |
| 26:YB:8:U:H3 | 26:YB:112:G:H1 | 1.52 | 0.58 |
| 29:YF:39:TRP:NE1 | 29:YF:99:TYR:O | 2.32 | 0.58 |
| 25:RA:1819:A:H5'' | 27:RD:161:THR:HG21 | 1.85 | 0.58 |
| 25:RA:270(S):G:H5' | 47:R1:76:ARG:HG2 | 1.86 | 0.58 |
| 40:RU:91:ASP:O | 40:RU:95:LEU:N | 2.35 | 0.58 |
| 1:XA:1141:C:H2' | 1:XA:1142:G:H8 | 1.69 | 0.58 |
| 1:XA:35:G:O2' | 12:XL:118:SER:O | 2.17 | 0.58 |
| 25:YA:2743:C:N1 | 55:Y9:26:ILE:HG12 | 2.19 | 0.58 |
| 25:YA:1464:C:HO2' | 25:YA:1528:A:H8 | 1.52 | 0.58 |
| 25:YA:813:U:H2' | 25:YA:814:C:H6 | 1.68 | 0.58 |
| 28:YE:24:THR:OG1 | 28:YE:186:GLY:HA2 | 2.03 | 0.58 |
| 1:QA:714:G:H2' | 1:QA:715:A:H8 | 1.66 | 0.58 |
| 25:RA:1656:C:H2' | 25:RA:1657:C:H6 | 1.69 | 0.58 |
| 25:RA:574:C:N3 | 28:RE:145:LYS:NZ | 2.38 | 0.58 |
| 1:XA:17:U:H2' | 1:XA:18:C:C6 | 2.39 | 0.58 |
| 1:XA:582:U:H5'' | 15:XO:64:ARG:HH12 | 1.69 | 0.58 |
| 5:XE:81:GLU:HG2 | 5:XE:90:VAL:HG22 | 1.86 | 0.58 |
| 13:XM:23:TYR:N | 13:XM:67:GLU:OE2 | 2.34 | 0.58 |
| 22:XV:59:A:O2' | 22:XV:61:U:OP2 | 2.12 | 0.58 |
| 25:YA:1613:G:O2' | 53:Y7:3:ARG:NE | 2.31 | 0.58 |
| 25:YA:458:G:O2' | 25:YA:469:G:O6 | 2.22 | 0.58 |
| 26:YB:24:G:O6 | 26:YB:56:G:O2' | 2.19 | 0.58 |
| 45:YZ:102:LEU:HD23 | 45:YZ:137:ILE:HB | 1.85 | 0.58 |
| 1:QA:181:G:O2' | 1:QA:182:U:O5' | 2.21 | 0.58 |
| 25:RA:1403:C:H5'' | 25:RA:1471:A:H1' | 1.85 | 0.58 |
| 25:RA:900:A:H3' | 25:RA:901:A:H8 | 1.68 | 0.58 |
| 28:RE:37:ARG:HD3 | 28:RE:42:ASP:OD2 | 2.03 | 0.58 |
| 20:XT:26:ASN:HB2 | 20:XT:71:THR:HG23 | 1.86 | 0.58 |
| 25:YA:2761:G:C2 | 25:YA:2762:G:H1' | 2.39 | 0.58 |
| 29:YF:156:LEU:HD21 | 29:YF:163:VAL:HG12 | 1.84 | 0.58 |
| 31:YH:164:TYR:HD2 | 31:YH:167:GLU:HB2 | 1.68 | 0.58 |
| 1:QA:1126:U:H1' | 1:QA:1280:A:N7 | 2.19 | 0.57 |
| 1:QA:1352:C:OP1 | 21:QU:3:LYS:NZ | 2.33 | 0.57 |
| 1:QA:17:U:H2' | 1:QA:18:C:H6 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:QV:15:G:H1 | 22:QV:49:C:H5 | 1.52 | 0.57 |
| 27:RD:31:LYS:HG3 | 27:RD:32:SER:H | 1.67 | 0.57 |
| 32:RI:4:ILE:HG12 | 32:RI:18:VAL:HG22 | 1.86 | 0.57 |
| 1:XA:269:C:H2' | 1:XA:270:A:C8 | 2.39 | 0.57 |
| 4:XD:127:THR:HA | 4:XD:132:ARG:HA | 1.85 | 0.57 |
| 8:XH:34:GLU:OE1 | 8:XH:37:ARG:NH2 | 2.37 | 0.57 |
| 12:XL:84:LEU:HB2 | 12:XL:105:TYR:CD2 | 2.39 | 0.57 |
| 25:YA:1416:G:H2' | 25:YA:1417:C:C6 | 2.39 | 0.57 |
| 25:YA:521:G:H2' | 25:YA:522:G:H8 | 1.68 | 0.57 |
| 11:QK:62:GLN:HG3 | 11:QK:97:ALA:HB2 | 1.86 | 0.57 |
| 37:RR:96:ARG:HH21 | 37:RR:117:VAL:HG23 | 1.69 | 0.57 |
| 12:XL:27:LEU:HD13 | 12:XL:62:SER:HB3 | 1.85 | 0.57 |
| 55:Y9:35:ARG:NH1 | 55:Y9:37:GLY:O | 2.36 | 0.57 |
| 25:YA:1173:G:N2 | 25:YA:1175:U:O4 | 2.37 | 0.57 |
| 25:YA:2046:G:H5' | 51:Y5:19:ARG:HG3 | 1.87 | 0.57 |
| 25:YA:2102:U:H2' | 25:YA:2103:C:H6 | 1.69 | 0.57 |
| 25:YA:775:G:H4' | 25:YA:776:G:H5' | 1.85 | 0.57 |
| 13:XM:3:ARG:HH12 | 30:YG:113:ARG:NH2 | 2.01 | 0.57 |
| 33:YN:6:PRO:HG3 | 33:YN:41:ASP:HB2 | 1.86 | 0.57 |
| 6:QF:95:GLU:O | 18:QR:32:ARG:NH1 | 2.37 | 0.57 |
| 20:QT:26:ASN:HA | 20:QT:29:LYS:HG2 | 1.86 | 0.57 |
| 48:R2:41:ILE:HD11 | 48:R2:44:LEU:HB2 | 1.86 | 0.57 |
| 25:RA:662:G:H2' | 25:RA:663:G:H8 | 1.70 | 0.57 |
| 25:RA:71:A:H62 | 25:RA:114:U:H1' | 1.68 | 0.57 |
| 25:RA:971:C:H2' | 25:RA:972:G:O4' | 2.04 | 0.57 |
| 40:RU:61:TRP:HB3 | 40:RU:93:LYS:O | 2.03 | 0.57 |
| 45:RZ:114:GLY:HA3 | 45:RZ:177:PRO:HG3 | 1.86 | 0.57 |
| 1:XA:976:G:OP2 | 1:XA:1358:U:O2' | 2.22 | 0.57 |
| 1:XA:261:U:OP2 | 20:XT:79:ARG:NH2 | 2.37 | 0.57 |
| 1:XA:62:U:H2' | 1:XA:63:C:C6 | 2.38 | 0.57 |
| 8:XH:106:GLY:O | 8:XH:122:ARG:NH2 | 2.36 | 0.57 |
| 47:Y1:85:LEU:HD12 | 47:Y1:88:LYS:HE3 | 1.84 | 0.57 |
| 25:YA:1310:G:OP2 | 53:Y7:9:ARG:NE | 2.30 | 0.57 |
| 25:YA:2743:C:C5' | 55:Y9:25:VAL:HA | 2.35 | 0.57 |
| 25:YA:2814:C:O2' | 51:Y5:29:THR:OG1 | 2.16 | 0.57 |
| 25:YA:307:G:N2 | 25:YA:310:A:OP2 | 2.37 | 0.57 |
| 25:YA:259:G:O2' | 25:YA:621:A:O2' | 2.11 | 0.57 |
| 25:YA:629:G:N3 | 25:YA:639:U:O2' | 2.37 | 0.57 |
| 1:QA:737:A:H2' | 1:QA:738:C:C6 | 2.39 | 0.57 |
| 11:QK:33:THR:HG22 | 11:QK:39:PRO:HA | 1.86 | 0.57 |
| 22:QW:8:U:C2 | 22:QW:14:A:N7 | 2.71 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:RQ:83:MET:HE3 | 46:R0:7:LEU:HB2 | 1.86 | 0.57 |
| 25:RA:1518:C:H2' | 25:RA:1519:G:C8 | 2.38 | 0.57 |
| 25:RA:855:G:H1 | 25:RA:922:U:H3 | 1.50 | 0.57 |
| 32:RI:80:PRO:HB2 | 32:RI:146:ALA:HB2 | 1.86 | 0.57 |
| 25:RA:2250:G:C4 | 36:RQ:82:ARG:HG3 | 2.39 | 0.57 |
| 40:RU:91:ASP:O | 40:RU:93:LYS:N | 2.38 | 0.57 |
| 1:XA:1213:A:N6 | 1:XA:1215:G:N3 | 2.52 | 0.57 |
| 1:XA:1224:G:O2' | 1:XA:1322:C:OP2 | 2.22 | 0.57 |
| 1:XA:363:A:OP1 | 12:XL:34:ARG:N | 2.28 | 0.57 |
| 25:YA:1165:U:H2' | 25:YA:1166:C:C6 | 2.39 | 0.57 |
| 25:YA:1791:A:H3' | 25:YA:1792:G:H8 | 1.69 | 0.57 |
| 25:YA:2743:C:H3' | 55:Y9:24:TYR:O | 2.03 | 0.57 |
| 45:YZ:102:LEU:HD11 | 45:YZ:124:ILE:HG13 | 1.85 | 0.57 |
| 1:QA:1218:C:H2' | 1:QA:1219:U:C6 | 2.39 | 0.57 |
| 25:RA:1262:A:OP1 | 42:RW:99:ARG:NH1 | 2.33 | 0.57 |
| 25:RA:220:G:H21 | 25:RA:429:A:H62 | 1.50 | 0.57 |
| 39:RT:51:ARG:HG2 | 39:RT:98:LYS:HE3 | 1.85 | 0.57 |
| 13:XM:52:GLU:HG2 | 13:XM:55:ARG:HH21 | 1.68 | 0.57 |
| 22:XW:17:C:OP1 | 22:XW:61:U:O2' | 2.20 | 0.57 |
| 25:YA:1333:C:H2' | 25:YA:1334:G:H8 | 1.70 | 0.57 |
| 25:YA:514:A:N3 | 25:YA:581:C:O2' | 2.33 | 0.57 |
| 32:YI:121:LYS:HG2 | 32:YI:122:GLU:H | 1.70 | 0.57 |
| 1:QA:1507:A:H2' | 1:QA:1508:G:C8 | 2.39 | 0.57 |
| 22:XV:44:A:H2' | 22:XV:45:A:H8 | 1.70 | 0.57 |
| 27:YD:231:HIS:CD2 | 27:YD:249:PRO:HG3 | 2.39 | 0.57 |
| 1:QA:1321:C:H3' | 1:QA:1322:C:H5'' | 1.85 | 0.57 |
| 1:QA:1342:C:H2' | 1:QA:1343:G:C8 | 2.39 | 0.57 |
| 1:QA:501:C:H2' | 1:QA:502:G:H8 | 1.69 | 0.57 |
| 25:RA:1796:U:H2' | 25:RA:1797:C:H6 | 1.69 | 0.57 |
| 25:RA:2752:C:H3' | 25:RA:2753:A:C8 | 2.40 | 0.57 |
| 25:RA:2836:U:H2' | 25:RA:2837:G:C8 | 2.38 | 0.57 |
| 1:XA:243:A:H4' | 1:XA:244:U:O5' | 2.03 | 0.57 |
| 25:YA:1116:C:H2' | 25:YA:1117:G:C8 | 2.38 | 0.57 |
| 25:YA:1353:A:H2' | 25:YA:1354:A:C8 | 2.40 | 0.57 |
| 25:YA:2747:G:C6 | 25:YA:2755:C:H4' | 2.40 | 0.57 |
| 25:YA:414:C:O2 | 25:YA:1864:U:O2' | 2.22 | 0.57 |
| 25:YA:823:G:H2' | 25:YA:824:A:H8 | 1.68 | 0.57 |
| 36:YQ:32:TYR:CE1 | 36:YQ:133:ARG:HG3 | 2.39 | 0.57 |
| 9:QI:17:VAL:HG11 | 9:QI:81:ILE:HD13 | 1.87 | 0.57 |
| 46:R0:23:VAL:HG13 | 46:R0:38:VAL:HG22 | 1.86 | 0.57 |
| 32:RI:27:ARG:HB2 | 47:R1:71:TYR:CE2 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:RO:23:ARG:NH2 | 34:RO:28:SER:O | 2.37 | 0.57 |
| 9:XI:17:VAL:HG11 | 9:XI:81:ILE:HD13 | 1.87 | 0.57 |
| 17:XQ:28:PRO:HA | 17:XQ:35:VAL:HA | 1.85 | 0.57 |
| 25:YA:1796:U:H2' | 25:YA:1797:C:H6 | 1.68 | 0.57 |
| 25:YA:2103:C:H2' | 25:YA:2104:G:C8 | 2.39 | 0.57 |
| 35:YP:106:LEU:HD21 | 35:YP:112:LEU:HD13 | 1.87 | 0.57 |
| 35:YP:63:PRO:HB3 | 54:Y8:13:ARG:HB3 | 1.85 | 0.57 |
| 1:QA:316:G:OP2 | 1:QA:351:G:O2' | 2.21 | 0.57 |
| 1:QA:34:C:H2' | 1:QA:35:G:H8 | 1.70 | 0.57 |
| 25:RA:1169:G:H1 | 25:RA:1180:C:H42 | 1.53 | 0.57 |
| 25:RA:1266:G:O6 | 42:RW:13:SER:OG | 2.15 | 0.57 |
| 27:RD:34:VAL:O | 27:RD:35:LYS:HG2 | 2.05 | 0.57 |
| 36:RQ:81:VAL:HG23 | 36:RQ:82:ARG:H | 1.69 | 0.57 |
| 25:RA:994:C:H3' | 40:RU:54:LYS:HE3 | 1.86 | 0.57 |
| 1:XA:1336:C:O2 | 1:XA:1337:G:N1 | 2.38 | 0.57 |
| 1:XA:22:G:H4' | 1:XA:885:G:C8 | 2.40 | 0.57 |
| 1:XA:701:C:O2 | 1:XA:703:G:N1 | 2.38 | 0.57 |
| 1:XA:191:G:C4 | 20:XT:105:SER:HB3 | 2.39 | 0.57 |
| 22:XW:8:U:H4' | 22:XW:9:G:OP1 | 2.05 | 0.57 |
| 25:YA:2762:G:H1 | 55:Y9:33:LYS:HZ3 | 1.51 | 0.57 |
| 25:YA:1508:A:O2' | 25:YA:1509:C:O4' | 2.23 | 0.57 |
| 25:YA:1999:C:OP1 | 25:YA:2723:C:O2' | 2.22 | 0.57 |
| 25:YA:309:G:N3 | 25:YA:329:G:O2' | 2.38 | 0.57 |
| 42:YW:86:LEU:HD22 | 42:YW:96:ILE:HD11 | 1.85 | 0.57 |
| 1:QA:1064:G:H1' | 1:QA:1066:C:C6 | 2.40 | 0.57 |
| 1:QA:1314:C:H2' | 1:QA:1315:U:C6 | 2.40 | 0.57 |
| 50:R4:56:VAL:HG23 | 50:R4:58:ARG:HG3 | 1.86 | 0.57 |
| 25:RA:1316:U:H2' | 25:RA:1317:A:H8 | 1.70 | 0.57 |
| 33:RN:70:LYS:HD3 | 33:RN:87:LEU:HD12 | 1.86 | 0.57 |
| 35:RP:84:ASN:HA | 35:RP:115:LEU:O | 2.05 | 0.57 |
| 1:XA:410:G:H2' | 1:XA:429:U:C5 | 2.40 | 0.57 |
| 9:XI:10:ARG:HE | 9:XI:105:ASP:HB2 | 1.70 | 0.57 |
| 47:Y1:50:ARG:HD2 | 47:Y1:57:GLU:OE2 | 2.05 | 0.57 |
| 25:YA:1081:U:H3' | 25:YA:1082:U:H4' | 1.87 | 0.57 |
| 25:YA:581:C:H2' | 25:YA:582:G:C8 | 2.40 | 0.57 |
| 1:QA:1123:A:H4' | 10:QJ:36:GLY:HA3 | 1.87 | 0.56 |
| 29:RF:63:LYS:NZ | 29:RF:75:HIS:O | 2.30 | 0.56 |
| 45:RZ:163:LEU:HD22 | 45:RZ:167:PRO:HG3 | 1.87 | 0.56 |
| 1:XA:692:U:OP1 | 11:XK:124:LYS:NZ | 2.31 | 0.56 |
| 2:XB:77:ALA:HB2 | 2:XB:211:ILE:HD13 | 1.87 | 0.56 |
| 9:XI:5:TYR:CE1 | 9:XI:16:ARG:HB2 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1525:G:H2' | 25:YA:1526:G:H8 | 1.70 | 0.56 |
| 27:YD:231:HIS:HD2 | 27:YD:249:PRO:HG3 | 1.69 | 0.56 |
| 32:YI:88:ILE:HG22 | 32:YI:90:GLY:H | 1.69 | 0.56 |
| 36:YQ:63:LYS:HD2 | 45:YZ:175:VAL:HG21 | 1.86 | 0.56 |
| 1:QA:335:C:H2' | 1:QA:336:C:C6 | 2.40 | 0.56 |
| 1:QA:745:C:H2' | 1:QA:746:A:C8 | 2.39 | 0.56 |
| 3:QC:5:ILE:HD12 | 10:QJ:51:ARG:HH12 | 1.70 | 0.56 |
| 8:QH:17:THR:O | 8:QH:78:GLN:NE2 | 2.38 | 0.56 |
| 35:RP:96:THR:HG22 | 35:RP:126:VAL:HB | 1.88 | 0.56 |
| 39:RT:3:ARG:HG3 | 39:RT:7:ILE:HG12 | 1.86 | 0.56 |
| 1:XA:618:C:H5' | 1:XA:619:U:H5'' | 1.86 | 0.56 |
| 25:YA:212:G:H2' | 25:YA:213:A:C8 | 2.41 | 0.56 |
| 27:YD:44:ASN:HB3 | 27:YD:49:ILE:HA | 1.86 | 0.56 |
| 32:YI:82:ARG:HA | 32:YI:145:VAL:HG12 | 1.87 | 0.56 |
| 28:YE:19:ARG:HG3 | 34:YO:72:PRO:HB2 | 1.88 | 0.56 |
| 37:YR:79:LEU:HD12 | 37:YR:83:ILE:HB | 1.86 | 0.56 |
| 1:QA:769:G:H4' | 1:QA:1513:A:H4' | 1.86 | 0.56 |
| 1:QA:352:C:O2' | 1:QA:354:G:OP1 | 2.18 | 0.56 |
| 1:QA:1100:C:P | 2:QB:96:ARG:HD3 | 2.45 | 0.56 |
| 25:RA:1198:U:H2' | 25:RA:1199:U:H6 | 1.70 | 0.56 |
| 25:RA:1224:G:OP2 | 41:RV:66:ARG:NH1 | 2.36 | 0.56 |
| 25:RA:1438:U:H2' | 25:RA:1439:A:H8 | 1.69 | 0.56 |
| 25:RA:1509:C:H3' | 25:RA:1510:A:H5'' | 1.87 | 0.56 |
| 25:RA:1796:U:H2' | 25:RA:1797:C:C6 | 2.40 | 0.56 |
| 25:RA:2126:A:N6 | 25:RA:2163:C:O2' | 2.37 | 0.56 |
| 25:RA:38:A:H2' | 25:RA:39:C:C6 | 2.39 | 0.56 |
| 25:RA:848:G:H2' | 25:RA:849:A:C8 | 2.41 | 0.56 |
| 1:XA:890:G:O2' | 1:XA:906:G:O6 | 2.20 | 0.56 |
| 1:XA:1235:U:H5'' | 21:XU:3:LYS:HD2 | 1.87 | 0.56 |
| 54:Y8:29:LYS:HB2 | 54:Y8:33:ASN:HD21 | 1.70 | 0.56 |
| 27:YD:62:TYR:HA | 27:YD:87:ASN:ND2 | 2.19 | 0.56 |
| 29:YF:116:ASP:OD2 | 35:YP:1:MET:N | 2.36 | 0.56 |
| 30:YG:142:PRO:HB2 | 50:Y4:31:ILE:HG21 | 1.87 | 0.56 |
| 31:YH:83:TYR:CE2 | 31:YH:138:LYS:HD2 | 2.41 | 0.56 |
| 1:QA:418:C:H2' | 1:QA:419:C:C6 | 2.40 | 0.56 |
| 4:QD:13:ARG:HH21 | 4:QD:40:PRO:HB3 | 1.69 | 0.56 |
| 25:RA:2368:C:H2' | 25:RA:2369:A:H8 | 1.69 | 0.56 |
| 25:RA:969:U:H2' | 25:RA:970:C:C6 | 2.40 | 0.56 |
| 25:RA:617:G:OP1 | 29:RF:40:GLN:HG3 | 2.06 | 0.56 |
| 35:RP:97:PRO:O | 35:RP:98:GLU:HG2 | 2.05 | 0.56 |
| 37:RR:100:LEU:HD11 | 37:RR:113:LEU:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:RX:12:VAL:HB | 43:RX:27:THR:HG23 | 1.87 | 0.56 |
| 1:XA:1077:G:N2 | 1:XA:1080:A:OP2 | 2.27 | 0.56 |
| 1:XA:1446:A:O2' | 1:XA:1447:G:O5' | 2.22 | 0.56 |
| 1:XA:250:A:H4' | 1:XA:251:G:O5' | 2.05 | 0.56 |
| 27:YD:142:VAL:HG23 | 27:YD:193:VAL:HA | 1.88 | 0.56 |
| 31:YH:43:VAL:HG22 | 31:YH:52:VAL:HG22 | 1.87 | 0.56 |
| 31:YH:8:PRO:CG | 31:YH:69:ARG:HE | 2.17 | 0.56 |
| 1:QA:156:G:H2' | 1:QA:157:G:H8 | 1.71 | 0.56 |
| 1:QA:718:G:N2 | 18:QR:49:LYS:HG2 | 2.20 | 0.56 |
| 12:QL:86:ARG:HB2 | 12:QL:101:VAL:HG23 | 1.87 | 0.56 |
| 1:QA:750:G:N3 | 15:QO:23:GLY:HA3 | 2.20 | 0.56 |
| 25:RA:1103:A:H5'' | 25:RA:1104:C:H5 | 1.71 | 0.56 |
| 25:RA:2246:G:H2' | 25:RA:2247:A:C8 | 2.40 | 0.56 |
| 1:XA:339:C:OP1 | 34:YO:13:ASN:ND2 | 2.34 | 0.56 |
| 1:XA:963:G:H21 | 10:XJ:55:LYS:HD3 | 1.69 | 0.56 |
| 11:XK:41:THR:HG21 | 11:XK:71:LYS:HB3 | 1.86 | 0.56 |
| 25:YA:1417:C:H2' | 25:YA:1418:G:O4' | 2.06 | 0.56 |
| 25:YA:270(I):G:H1 | 25:YA:270(Q):C:H42 | 1.54 | 0.56 |
| 25:YA:2822:G:O2' | 25:YA:2825:C:N4 | 2.35 | 0.56 |
| 25:YA:372:G:N2 | 25:YA:401:A:OP2 | 2.39 | 0.56 |
| 25:YA:547:A:H2' | 25:YA:548:A:C8 | 2.40 | 0.56 |
| 27:YD:146:GLU:HB2 | 27:YD:189:CYS:HB3 | 1.88 | 0.56 |
| 1:QA:337:C:H2' | 1:QA:338:A:H8 | 1.70 | 0.56 |
| 1:QA:890:G:O2' | 1:QA:906:G:O6 | 2.17 | 0.56 |
| 25:RA:1005:C:O2' | 33:RN:28:THR:HG21 | 2.05 | 0.56 |
| 25:RA:1535:U:H5'' | 25:RA:1537:C:N3 | 2.20 | 0.56 |
| 25:RA:2219:G:OP1 | 27:RD:172:TYR:OH | 2.19 | 0.56 |
| 25:RA:2355:C:H4' | 46:R0:24:LYS:HG3 | 1.87 | 0.56 |
| 3:XC:95:THR:HG22 | 3:XC:97:LYS:H | 1.71 | 0.56 |
| 25:YA:1571:A:H2' | 25:YA:1572:A:H8 | 1.70 | 0.56 |
| 25:YA:2037:G:H2' | 25:YA:2038:G:C8 | 2.40 | 0.56 |
| 25:YA:226:G:H2' | 25:YA:227:A:C8 | 2.41 | 0.56 |
| 1:QA:119:A:H4' | 1:QA:120:A:O5' | 2.04 | 0.56 |
| 49:R3:15:TYR:HE2 | 49:R3:53:LEU:HD21 | 1.69 | 0.56 |
| 25:RA:2394:C:OP1 | 35:RP:63:PRO:HD2 | 2.06 | 0.56 |
| 3:XC:150:LYS:HE2 | 3:XC:152:ILE:HD11 | 1.88 | 0.56 |
| 25:YA:2741:A:N7 | 55:Y9:30:PRO:HB2 | 2.21 | 0.56 |
| 25:YA:949:C:H2' | 25:YA:950:G:H8 | 1.71 | 0.56 |
| 27:YD:85:ASP:OD2 | 27:YD:88:ARG:NH1 | 2.35 | 0.56 |
| 1:QA:1292:U:H2' | 1:QA:1293:G:H8 | 1.71 | 0.56 |
| 1:QA:406:G:H2' | 1:QA:407:G:H8 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:437:U:H2' | 1:QA:438:G:O4' | 2.06 | 0.56 |
| 13:QM:49:THR:HG22 | 13:QM:51:ALA:H | 1.70 | 0.56 |
| 25:RA:1490:A:O2' | 27:RD:99:ASP:OD1 | 2.24 | 0.56 |
| 25:RA:2197:U:H1' | 25:RA:2198:A:C8 | 2.40 | 0.56 |
| 25:RA:2241:A:H2' | 25:RA:2242:G:C8 | 2.40 | 0.56 |
| 25:RA:50:U:H3' | 25:RA:51:G:H5' | 1.86 | 0.56 |
| 44:RY:14:LEU:HB2 | 44:RY:75:ILE:HD11 | 1.87 | 0.56 |
| 2:XB:24:TRP:CZ3 | 2:XB:26:PRO:HA | 2.40 | 0.56 |
| 19:XS:32:LYS:HA | 19:XS:50:ALA:HB3 | 1.88 | 0.56 |
| 25:YA:2747:G:H4' | 31:YH:70:THR:HB | 1.88 | 0.56 |
| 25:YA:2837:G:H2' | 25:YA:2838:G:H8 | 1.71 | 0.56 |
| 27:YD:260:ARG:NH2 | 27:YD:264:LYS:HD3 | 2.20 | 0.56 |
| 28:YE:23:VAL:HG12 | 28:YE:173:VAL:HG21 | 1.88 | 0.56 |
| 33:YN:12:ARG:HH11 | 33:YN:14:VAL:HG22 | 1.71 | 0.56 |
| 40:YU:81:HIS:NE2 | 40:YU:85:LYS:HE3 | 2.21 | 0.56 |
| 14:QN:29:ARG:HD3 | 14:QN:40:CYS:HB2 | 1.86 | 0.56 |
| 25:RA:37:C:H2' | 25:RA:38:A:C8 | 2.41 | 0.56 |
| 25:RA:574:C:N4 | 25:RA:2034:U:OP1 | 2.38 | 0.56 |
| 25:RA:822:U:H2' | 25:RA:823:G:H8 | 1.70 | 0.56 |
| 27:RD:133:LEU:HB3 | 27:RD:173:VAL:HG21 | 1.88 | 0.56 |
| 1:XA:56:U:H2' | 1:XA:57:G:C8 | 2.41 | 0.56 |
| 1:XA:736:C:H2' | 1:XA:737:A:H8 | 1.71 | 0.56 |
| 7:XG:116:ALA:HA | 7:XG:119:ARG:HE | 1.71 | 0.56 |
| 9:XI:5:TYR:HE1 | 9:XI:16:ARG:HB2 | 1.71 | 0.56 |
| 12:XL:83:VAL:HG13 | 12:XL:100:ILE:HG23 | 1.88 | 0.56 |
| 25:YA:2469:A:H5'' | 25:YA:2470:G:C8 | 2.41 | 0.56 |
| 25:YA:836:G:H2' | 25:YA:837:C:C6 | 2.41 | 0.56 |
| 30:YG:173:LEU:HD22 | 30:YG:178:PHE:CE2 | 2.41 | 0.56 |
| 37:YR:51:LEU:HD22 | 37:YR:66:VAL:HG13 | 1.88 | 0.56 |
| 44:YY:52:SER:HB2 | 44:YY:53:PRO:HD2 | 1.87 | 0.56 |
| 1:QA:80:G:H1 | 1:QA:89:U:H3 | 1.54 | 0.56 |
| 13:QM:15:VAL:HG22 | 13:QM:45:VAL:HB | 1.87 | 0.56 |
| 25:RA:2028:U:H2' | 25:RA:2029:G:C8 | 2.41 | 0.56 |
| 25:RA:2103:C:H2' | 25:RA:2104:G:C8 | 2.41 | 0.56 |
| 27:RD:62:TYR:HA | 27:RD:87:ASN:ND2 | 2.20 | 0.56 |
| 30:RG:161:THR:HG22 | 30:RG:163:ALA:H | 1.69 | 0.56 |
| 1:XA:1321:C:H3' | 1:XA:1322:C:H5'' | 1.87 | 0.56 |
| 1:XA:21:G:H2' | 1:XA:22:G:C8 | 2.40 | 0.56 |
| 25:YA:2638:G:OP1 | 28:YE:82:ARG:NH2 | 2.39 | 0.56 |
| 25:YA:2853:C:H2' | 25:YA:2854:G:H8 | 1.70 | 0.56 |
| 37:YR:74:LYS:C | 37:YR:76:VAL:H | 2.09 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:YU:36:ARG:HG2 | 40:YU:40:PHE:CE2 | 2.41 | 0.56 |
| 1:QA:985:C:H2' | 1:QA:986:A:C8 | 2.41 | 0.56 |
| 25:RA:1209:G:O2' | 25:RA:1237:A:N1 | 2.37 | 0.56 |
| 25:RA:2064:C:H2' | 25:RA:2065:C:C6 | 2.40 | 0.56 |
| 25:RA:270(N):G:OP1 | 32:RI:57:ARG:NH1 | 2.39 | 0.56 |
| 25:RA:2852:G:H1 | 25:RA:2865:U:H3 | 1.53 | 0.56 |
| 25:RA:65:C:H1' | 25:RA:456:C:H42 | 1.71 | 0.56 |
| 27:RD:32:SER:HA | 27:RD:35:LYS:HB2 | 1.88 | 0.56 |
| 28:RE:55:ASN:ND2 | 28:RE:75:VAL:HG22 | 2.21 | 0.56 |
| 33:RN:34:LEU:O | 33:RN:49:GLY:HA3 | 2.06 | 0.56 |
| 1:XA:1296:C:H1' | 1:XA:1302:U:H5 | 1.70 | 0.56 |
| 1:XA:452:A:H62 | 1:XA:480:U:H3 | 1.54 | 0.56 |
| 4:XD:50:ARG:HD2 | 4:XD:51:PRO:HD2 | 1.88 | 0.56 |
| 15:XO:15:PHE:HE2 | 15:XO:85:LEU:HD21 | 1.71 | 0.56 |
| 25:YA:1203:G:H3' | 25:YA:1204:A:H5'' | 1.88 | 0.56 |
| 25:YA:1571:A:H2' | 25:YA:1572:A:C8 | 2.41 | 0.56 |
| 25:YA:249:C:O2 | 54:Y8:12:LYS:NZ | 2.37 | 0.56 |
| 25:YA:2740:A:N6 | 25:YA:2764:A:N7 | 2.53 | 0.56 |
| 25:YA:593:G:H2' | 25:YA:594:U:C6 | 2.41 | 0.56 |
| 28:YE:36:ARG:HH12 | 28:YE:86:PRO:HD2 | 1.71 | 0.56 |
| 34:YO:68:GLU:HG3 | 34:YO:78:ARG:HD3 | 1.88 | 0.56 |
| 25:YA:567:A:O3' | 35:YP:36:LYS:NZ | 2.39 | 0.56 |
| 1:QA:337:C:H2' | 1:QA:338:A:C8 | 2.39 | 0.55 |
| 1:QA:362:G:N2 | 1:QA:365:U:OP2 | 2.39 | 0.55 |
| 1:QA:501:C:H2' | 1:QA:502:G:C8 | 2.41 | 0.55 |
| 11:QK:83:ILE:HG12 | 11:QK:109:VAL:HG22 | 1.87 | 0.55 |
| 11:QK:109:VAL:HG12 | 18:QR:86:VAL:HA | 1.87 | 0.55 |
| 25:RA:582:G:H2' | 25:RA:583:G:H8 | 1.71 | 0.55 |
| 28:RE:23:VAL:HG21 | 28:RE:183:LEU:HD23 | 1.88 | 0.55 |
| 36:RQ:29:PHE:N | 36:RQ:105:GLU:OE2 | 2.27 | 0.55 |
| 4:XD:54:TYR:HE1 | 4:XD:209:ARG:HH12 | 1.53 | 0.55 |
| 22:XV:35:C:H2' | 22:XV:36:A:C8 | 2.41 | 0.55 |
| 55:Y9:21:GLY:C | 55:Y9:22:ARG:HD2 | 2.26 | 0.55 |
| 25:YA:1652:A:OP1 | 37:YR:8:ARG:NH1 | 2.37 | 0.55 |
| 25:YA:588:U:H2' | 25:YA:589:C:C6 | 2.41 | 0.55 |
| 25:YA:679:C:H2' | 25:YA:680:G:C8 | 2.41 | 0.55 |
| 29:YF:70:THR:HG23 | 29:YF:72:ARG:H | 1.71 | 0.55 |
| 1:QA:1279:A:O2' | 1:QA:1282:C:N4 | 2.39 | 0.55 |
| 1:QA:344:A:O2' | 1:QA:346:G:O6 | 2.24 | 0.55 |
| 1:QA:891:U:H2' | 1:QA:892:A:H8 | 1.70 | 0.55 |
| 16:QP:4:ILE:HB | 16:QP:66:PRO:HB3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2591:C:H2' | 25:RA:2592:G:C8 | 2.41 | 0.55 |
| 31:RH:107:VAL:HB | 31:RH:153:LYS:NZ | 2.22 | 0.55 |
| 39:RT:123:GLN:O | 39:RT:126:ALA:N | 2.38 | 0.55 |
| 25:RA:996:A:H4' | 40:RU:92:ARG:HG2 | 1.88 | 0.55 |
| 1:XA:1516:G:N2 | 1:XA:1519:A:OP2 | 2.34 | 0.55 |
| 25:YA:994:C:OP1 | 40:YU:53:ARG:NH2 | 2.39 | 0.55 |
| 25:YA:2052:G:H4' | 28:YE:143:ASN:O | 2.06 | 0.55 |
| 35:YP:30:THR:O | 35:YP:33:ARG:HG2 | 2.05 | 0.55 |
| 25:YA:336:C:H4' | 44:YY:6:HIS:CD2 | 2.41 | 0.55 |
| 1:QA:674:G:H2' | 1:QA:675:A:H8 | 1.69 | 0.55 |
| 25:RA:247:G:H4' | 25:RA:386:G:C5 | 2.40 | 0.55 |
| 25:RA:2789:C:N4 | 25:RA:2894:G:O6 | 2.38 | 0.55 |
| 25:RA:709:U:H2' | 25:RA:710:G:H8 | 1.70 | 0.55 |
| 30:RG:19:LEU:HD11 | 30:RG:172:LEU:HD13 | 1.88 | 0.55 |
| 1:XA:885:G:H2' | 1:XA:886:G:H8 | 1.71 | 0.55 |
| 25:YA:2241:A:H2' | 25:YA:2242:G:C8 | 2.42 | 0.55 |
| 25:YA:2502:G:H5'' | 25:YA:2503:A:H5'' | 1.88 | 0.55 |
| 25:YA:1423:G:H5'' | 27:YD:33:LEU:HD11 | 1.87 | 0.55 |
| 31:YH:88:LEU:HA | 31:YH:130:ARG:HA | 1.88 | 0.55 |
| 1:QA:45:U:H2' | 1:QA:46:G:C8 | 2.41 | 0.55 |
| 1:QA:55:A:N6 | 1:QA:356:A:N1 | 2.53 | 0.55 |
| 1:QA:737:A:H2' | 1:QA:738:C:H6 | 1.72 | 0.55 |
| 25:RA:1543:A:O2' | 25:RA:1544:C:H3' | 2.06 | 0.55 |
| 25:RA:184:C:H2' | 25:RA:185:U:C6 | 2.41 | 0.55 |
| 25:RA:2076:U:OP2 | 25:RA:2238:G:N2 | 2.39 | 0.55 |
| 25:RA:856:C:O2' | 25:RA:857:C:OP1 | 2.21 | 0.55 |
| 30:RG:170:ARG:NH2 | 30:RG:182:LYS:O | 2.38 | 0.55 |
| 1:XA:1244:C:H2' | 1:XA:1245:A:C8 | 2.41 | 0.55 |
| 1:XA:1314:C:OP1 | 19:XS:6:LYS:HE3 | 2.07 | 0.55 |
| 1:XA:1414:U:H2' | 1:XA:1415:G:H8 | 1.71 | 0.55 |
| 1:XA:309:G:H2' | 1:XA:310:G:H8 | 1.71 | 0.55 |
| 1:XA:674:G:H2' | 1:XA:675:A:C8 | 2.40 | 0.55 |
| 1:XA:708:C:H2' | 1:XA:709:G:H8 | 1.70 | 0.55 |
| 11:XK:29:ILE:HG13 | 11:XK:44:SER:HB3 | 1.89 | 0.55 |
| 25:YA:2020:A:H5' | 51:Y5:12:SER:HB3 | 1.88 | 0.55 |
| 25:YA:1264:G:OP1 | 51:Y5:19:ARG:NH2 | 2.38 | 0.55 |
| 25:YA:1155:A:OP1 | 40:YU:55:ARG:HD2 | 2.06 | 0.55 |
| 25:YA:1196:C:HO2' | 25:YA:1228:G:HO2' | 1.46 | 0.55 |
| 25:YA:1438:U:H2' | 25:YA:1439:A:H8 | 1.71 | 0.55 |
| 25:YA:2123:G:H2' | 25:YA:2124:G:H8 | 1.71 | 0.55 |
| 25:YA:305:U:H2' | 25:YA:306:U:C6 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:YT:121:ILE:O | 39:YT:125:ARG:HG2 | 2.06 | 0.55 |
| 2:QB:51:LEU:HD23 | 2:QB:201:ILE:HD12 | 1.88 | 0.55 |
| 48:R2:14:ARG:NH1 | 48:R2:66:GLU:OE1 | 2.40 | 0.55 |
| 25:RA:2298:A:H62 | 25:RA:2318:G:H8 | 1.53 | 0.55 |
| 32:RI:100:ALA:O | 32:RI:104:GLN:HB3 | 2.05 | 0.55 |
| 25:RA:2845:G:OP1 | 39:RT:56:GLY:N | 2.39 | 0.55 |
| 1:XA:1435:G:H2' | 1:XA:1436:U:C6 | 2.41 | 0.55 |
| 1:XA:45:U:H2' | 1:XA:46:G:C8 | 2.42 | 0.55 |
| 12:XL:33:ARG:H | 12:XL:85:ILE:HG22 | 1.69 | 0.55 |
| 22:XW:5:G:H2' | 22:XW:6:G:H8 | 1.72 | 0.55 |
| 25:YA:1902:C:H5' | 27:YD:246:PRO:HD3 | 1.87 | 0.55 |
| 25:YA:208:C:H2' | 25:YA:209:C:H6 | 1.72 | 0.55 |
| 25:YA:2867:G:OP2 | 39:YT:119:LYS:NZ | 2.30 | 0.55 |
| 34:YO:2:ILE:HB | 34:YO:33:ALA:HB3 | 1.88 | 0.55 |
| 39:YT:123:GLN:O | 39:YT:125:ARG:N | 2.40 | 0.55 |
| 1:QA:864:A:H2' | 1:QA:865:A:C8 | 2.41 | 0.55 |
| 1:QA:707:C:H4' | 11:QK:20:TYR:CD2 | 2.42 | 0.55 |
| 22:QW:8:U:H4' | 22:QW:9:G:OP1 | 2.06 | 0.55 |
| 25:RA:2258:C:O2' | 25:RA:2427:C:OP2 | 2.23 | 0.55 |
| 25:RA:392:C:H5'' | 25:RA:409:C:H5'' | 1.88 | 0.55 |
| 25:RA:589:C:H2' | 25:RA:590:A:C8 | 2.41 | 0.55 |
| 39:RT:101:PHE:HD2 | 39:RT:105:LEU:HD21 | 1.71 | 0.55 |
| 1:XA:712:A:H2' | 1:XA:713:G:C8 | 2.41 | 0.55 |
| 3:XC:19:GLU:HG2 | 3:XC:54:ARG:HE | 1.71 | 0.55 |
| 53:Y7:5:TRP:NE1 | 53:Y7:7:PRO:HG3 | 2.22 | 0.55 |
| 25:YA:151:C:H2' | 25:YA:152:G:H8 | 1.71 | 0.55 |
| 26:YB:28:C:H2' | 26:YB:29:A:C8 | 2.42 | 0.55 |
| 1:QA:1013:G:N2 | 1:QA:1016:A:OP2 | 2.32 | 0.55 |
| 1:QA:816:A:OP1 | 1:QA:1526:G:O2' | 2.23 | 0.55 |
| 2:QB:58:ILE:HD11 | 2:QB:185:ILE:HD13 | 1.88 | 0.55 |
| 1:QA:581:G:O3' | 15:QO:64:ARG:NH2 | 2.39 | 0.55 |
| 25:RA:1080:C:N4 | 25:RA:1088:A:OP2 | 2.30 | 0.55 |
| 25:RA:2618:G:H21 | 28:RE:150:VAL:HG21 | 1.70 | 0.55 |
| 1:XA:1412:C:H2' | 1:XA:1413:A:C8 | 2.41 | 0.55 |
| 2:XB:51:LEU:HD23 | 2:XB:201:ILE:HD12 | 1.88 | 0.55 |
| 13:XM:49:THR:HG22 | 13:XM:51:ALA:H | 1.71 | 0.55 |
| 19:XS:15:LEU:H | 19:XS:15:LEU:HD23 | 1.71 | 0.55 |
| 50:Y4:14:ILE:HB | 50:Y4:22:ILE:HB | 1.88 | 0.55 |
| 53:Y7:12:ARG:NH2 | 53:Y7:44:PRO:HB3 | 2.22 | 0.55 |
| 25:YA:2535:G:H2' | 25:YA:2536:G:H8 | 1.71 | 0.55 |
| 25:YA:2591:C:H2' | 25:YA:2592:G:C8 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:278:A:H2' | 25:YA:279:C:C6 | 2.41 | 0.55 |
| 30:YG:161:THR:HG22 | 30:YG:163:ALA:H | 1.72 | 0.55 |
| 39:YT:19:LEU:HD22 | 39:YT:86:ILE:HG22 | 1.89 | 0.55 |
| 1:QA:360:A:H2' | 1:QA:361:G:C8 | 2.42 | 0.55 |
| 49:R3:39:ASP:OD1 | 49:R3:44:ARG:NH2 | 2.38 | 0.55 |
| 25:RA:774:A:OP1 | 27:RD:48:ARG:NH2 | 2.40 | 0.55 |
| 27:RD:69:ARG:NH2 | 27:RD:128:GLY:O | 2.29 | 0.55 |
| 38:RS:15:ARG:HG3 | 38:RS:19:LYS:HE2 | 1.89 | 0.55 |
| 8:XH:82:HIS:HB3 | 8:XH:138:TRP:CE2 | 2.42 | 0.55 |
| 22:XW:40:C:H2' | 22:XW:41:C:H6 | 1.72 | 0.55 |
| 25:YA:2081:C:H2' | 25:YA:2082:A:H8 | 1.71 | 0.55 |
| 31:YH:106:THR:HG22 | 31:YH:112:PRO:HB3 | 1.88 | 0.55 |
| 31:YH:149:ARG:C | 31:YH:151:ILE:H | 2.09 | 0.55 |
| 1:QA:1497:G:H1' | 1:QA:1518:A:H2 | 1.70 | 0.55 |
| 1:QA:407:G:H2' | 1:QA:408:A:H8 | 1.72 | 0.55 |
| 1:QA:405:U:O4 | 4:QD:2:GLY:N | 2.40 | 0.55 |
| 11:QK:21:ILE:HB | 11:QK:84:VAL:HG12 | 1.87 | 0.55 |
| 47:R1:6:GLU:O | 47:R1:91:LYS:HE3 | 2.07 | 0.55 |
| 50:R4:48:ARG:O | 50:R4:52:THR:OG1 | 2.25 | 0.55 |
| 32:RI:121:LYS:HG2 | 32:RI:122:GLU:H | 1.70 | 0.55 |
| 42:RW:57:ASN:O | 42:RW:61:ASN:HB2 | 2.07 | 0.55 |
| 1:XA:346:G:O2' | 1:XA:347:G:O5' | 2.25 | 0.55 |
| 1:XA:587:G:N2 | 1:XA:754:C:OP2 | 2.40 | 0.55 |
| 22:XW:28:U:H2' | 22:XW:29:C:H6 | 1.70 | 0.55 |
| 25:YA:1509:C:H3' | 25:YA:1510:A:H5'' | 1.89 | 0.55 |
| 25:YA:2754:U:H5' | 25:YA:2755:C:OP2 | 2.07 | 0.55 |
| 25:YA:768:G:O2' | 25:YA:1379:A:N6 | 2.39 | 0.55 |
| 27:YD:108:PRO:HB3 | 27:YD:143:HIS:CE1 | 2.42 | 0.55 |
| 1:QA:1096:C:H2' | 1:QA:1097:C:H6 | 1.71 | 0.55 |
| 1:QA:739:C:O2' | 15:QO:42:HIS:ND1 | 2.37 | 0.55 |
| 25:RA:1000:A:OP2 | 25:RA:1154:G:N1 | 2.35 | 0.55 |
| 25:RA:2746:U:H5'' | 31:RH:138:LYS:HE2 | 1.88 | 0.55 |
| 26:RB:32:C:N3 | 26:RB:51:G:N2 | 2.55 | 0.55 |
| 40:RU:90:VAL:HG12 | 40:RU:91:ASP:H | 1.71 | 0.55 |
| 25:YA:557:U:H2' | 25:YA:558:G:H8 | 1.71 | 0.55 |
| 35:YP:96:THR:HG22 | 35:YP:126:VAL:HB | 1.89 | 0.55 |
| 36:YQ:116:GLU:OE2 | 36:YQ:119:ARG:NH2 | 2.36 | 0.55 |
| 37:YR:24:GLN:HG3 | 37:YR:44:LEU:HD13 | 1.89 | 0.55 |
| 40:YU:92:ARG:HE | 41:YV:11:GLN:H | 1.55 | 0.55 |
| 43:YX:25:LYS:HB3 | 43:YX:80:ILE:HD11 | 1.88 | 0.55 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:H8 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:QH:83:ILE:HG13 | 8:QH:137:VAL:HG22 | 1.89 | 0.54 |
| 9:QI:116:LYS:HD3 | 9:QI:120:ARG:HA | 1.88 | 0.54 |
| 22:QV:15:G:H22 | 22:QV:49:C:H41 | 1.55 | 0.54 |
| 25:RA:1140:C:OP1 | 33:RN:23:LEU:HB3 | 2.06 | 0.54 |
| 25:RA:1290:C:H2' | 25:RA:1291:C:H6 | 1.72 | 0.54 |
| 25:RA:1681:G:O2' | 25:RA:1762:A:O2' | 2.20 | 0.54 |
| 25:RA:521:G:H2' | 25:RA:522:G:H8 | 1.71 | 0.54 |
| 30:RG:106:LEU:HD12 | 30:RG:110:ALA:HB3 | 1.88 | 0.54 |
| 30:RG:126:ASP:OD2 | 30:RG:130:ASN:HB2 | 2.08 | 0.54 |
| 34:RO:107:ARG:NH1 | 39:RT:36:GLU:OE1 | 2.40 | 0.54 |
| 35:RP:50:ARG:HB2 | 54:R8:59:LYS:HD3 | 1.88 | 0.54 |
| 1:XA:312:C:H2' | 1:XA:313:A:H8 | 1.72 | 0.54 |
| 1:XA:390:C:H2' | 1:XA:391:G:H8 | 1.72 | 0.54 |
| 8:XH:83:ILE:HG13 | 8:XH:137:VAL:HG22 | 1.89 | 0.54 |
| 25:YA:1055:G:H1 | 25:YA:1104:C:H42 | 1.53 | 0.54 |
| 25:YA:675:A:N3 | 25:YA:2443:C:O2' | 2.38 | 0.54 |
| 26:YB:28:C:H2' | 26:YB:29:A:H8 | 1.72 | 0.54 |
| 1:QA:1342:C:H2' | 1:QA:1343:G:H8 | 1.70 | 0.54 |
| 13:QM:54:VAL:HG22 | 13:QM:57:ARG:HH21 | 1.73 | 0.54 |
| 25:RA:226:G:O2' | 25:RA:228:A:N6 | 2.39 | 0.54 |
| 25:RA:2068:U:H3 | 25:RA:2430:A:H2 | 1.56 | 0.54 |
| 26:RB:28:C:H2' | 26:RB:29:A:H8 | 1.72 | 0.54 |
| 27:RD:231:HIS:HD2 | 27:RD:249:PRO:HG3 | 1.71 | 0.54 |
| 30:RG:129:GLY:O | 30:RG:161:THR:HB | 2.07 | 0.54 |
| 36:RQ:32:TYR:CE1 | 36:RQ:133:ARG:HG3 | 2.41 | 0.54 |
| 25:RA:2376:A:N6 | 38:RS:89:ARG:HD3 | 2.22 | 0.54 |
| 1:XA:1427:U:H2' | 1:XA:1428:A:H8 | 1.72 | 0.54 |
| 1:XA:946:A:H2' | 1:XA:947:G:C8 | 2.41 | 0.54 |
| 25:YA:172:C:H2' | 25:YA:173:G:C8 | 2.43 | 0.54 |
| 25:YA:320:A:H2' | 29:YF:136:THR:HG21 | 1.88 | 0.54 |
| 1:QA:139:G:H2' | 1:QA:140:A:H8 | 1.73 | 0.54 |
| 4:QD:197:PRO:HD3 | 6:XF:16:GLN:OE1 | 2.07 | 0.54 |
| 54:R8:26:LYS:HD2 | 54:R8:47:LYS:HD3 | 1.88 | 0.54 |
| 25:RA:1264:G:OP1 | 51:R5:19:ARG:NH2 | 2.35 | 0.54 |
| 25:RA:131:G:H2' | 25:RA:132:G:H8 | 1.73 | 0.54 |
| 25:RA:2246:G:H2' | 25:RA:2247:A:H8 | 1.72 | 0.54 |
| 25:RA:242:G:H4' | 25:RA:243:U:O5' | 2.07 | 0.54 |
| 25:RA:439:G:H2' | 25:RA:440:G:C8 | 2.42 | 0.54 |
| 25:RA:581:C:H2' | 25:RA:582:G:H8 | 1.72 | 0.54 |
| 35:RP:121:LYS:HD3 | 35:RP:122:PRO:HD2 | 1.89 | 0.54 |
| 39:RT:24:PRO:HA | 39:RT:49:VAL:HG13 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:994:C:OP1 | 40:RU:53:ARG:NH2 | 2.41 | 0.54 |
| 1:XA:56:U:H2' | 1:XA:57:G:H8 | 1.71 | 0.54 |
| 3:XC:108:ASN:HD21 | 3:XC:144:SER:HB2 | 1.73 | 0.54 |
| 50:Y4:48:ARG:O | 50:Y4:52:THR:OG1 | 2.25 | 0.54 |
| 25:YA:1525:G:H2' | 25:YA:1526:G:C8 | 2.42 | 0.54 |
| 25:YA:1791:A:H4' | 27:YD:206:LEU:HB2 | 1.89 | 0.54 |
| 25:YA:2591:C:H2' | 25:YA:2592:G:H8 | 1.73 | 0.54 |
| 25:YA:2705:A:O2' | 25:YA:2852:G:OP1 | 2.14 | 0.54 |
| 27:YD:34:VAL:O | 27:YD:35:LYS:HG2 | 2.07 | 0.54 |
| 29:YF:198:ALA:HA | 29:YF:201:VAL:HG12 | 1.89 | 0.54 |
| 36:YQ:24:GLY:H | 36:YQ:101:ARG:CD | 2.20 | 0.54 |
| 37:YR:28:LEU:HD23 | 37:YR:48:VAL:HG21 | 1.89 | 0.54 |
| 1:QA:436:C:H2' | 1:QA:437:U:C6 | 2.42 | 0.54 |
| 20:QT:26:ASN:HB2 | 20:QT:71:THR:HG23 | 1.89 | 0.54 |
| 22:QW:28:U:H2' | 22:QW:29:C:H6 | 1.72 | 0.54 |
| 25:RA:1936:A:H61 | 25:RA:1963:U:H3 | 1.55 | 0.54 |
| 25:RA:995:C:H5'' | 40:RU:54:LYS:HG2 | 1.88 | 0.54 |
| 45:RZ:30:ASN:OD1 | 45:RZ:33:LEU:N | 2.35 | 0.54 |
| 1:XA:1469:G:H2' | 1:XA:1470:G:H8 | 1.72 | 0.54 |
| 10:XJ:51:ARG:O | 14:XN:45:ARG:NH1 | 2.40 | 0.54 |
| 25:YA:1565:C:H5'' | 27:YD:18:VAL:HG11 | 1.90 | 0.54 |
| 25:YA:2151:G:H2' | 25:YA:2152:G:H8 | 1.72 | 0.54 |
| 25:YA:263:C:H2' | 25:YA:264:C:O4' | 2.07 | 0.54 |
| 25:YA:18:C:O2' | 25:YA:553:U:OP1 | 2.25 | 0.54 |
| 25:YA:2619:C:H5'' | 28:YE:152:LYS:HA | 1.88 | 0.54 |
| 43:YX:35:THR:HG23 | 43:YX:38:GLU:H | 1.72 | 0.54 |
| 25:YA:1334:G:H5'' | 43:YX:65:ARG:HH22 | 1.71 | 0.54 |
| 1:QA:1466:C:H2' | 1:QA:1467:G:O4' | 2.08 | 0.54 |
| 1:QA:489:C:H2' | 1:QA:490:G:H8 | 1.73 | 0.54 |
| 1:QA:738:C:H5'' | 6:QF:69:GLU:HB2 | 1.88 | 0.54 |
| 1:QA:1226:C:H42 | 13:QM:104:ARG:HH11 | 1.54 | 0.54 |
| 1:QA:1310:G:OP2 | 13:QM:88:ARG:NH2 | 2.41 | 0.54 |
| 22:QW:40:C:H2' | 22:QW:41:C:H6 | 1.73 | 0.54 |
| 25:RA:1802:A:H2' | 25:RA:1803:A:C8 | 2.43 | 0.54 |
| 26:RB:48:A:H2' | 26:RB:49:C:C6 | 2.43 | 0.54 |
| 1:XA:1345:U:OP1 | 9:XI:120:ARG:NH1 | 2.41 | 0.54 |
| 1:XA:971:G:N2 | 1:XA:1363:A:OP2 | 2.41 | 0.54 |
| 1:XA:1117:G:H4' | 9:XI:104:ARG:NH1 | 2.22 | 0.54 |
| 25:YA:1079:C:H2' | 25:YA:1080:C:C6 | 2.42 | 0.54 |
| 25:YA:1399:C:H2' | 25:YA:1400:G:H8 | 1.73 | 0.54 |
| 25:YA:1728:G:H8 | 25:YA:1732:A:H62 | 1.54 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2758:A:C5 | 31:YH:67:LEU:HD21 | 2.43 | 0.54 |
| 26:YB:111:U:H2' | 26:YB:112:G:H8 | 1.73 | 0.54 |
| 30:YG:82:LEU:HD21 | 30:YG:88:ILE:HG12 | 1.89 | 0.54 |
| 35:YP:122:PRO:HB3 | 35:YP:141:ALA:HB1 | 1.89 | 0.54 |
| 36:YQ:75:THR:HG21 | 36:YQ:85:LYS:HE3 | 1.88 | 0.54 |
| 1:QA:1120:G:H2' | 1:QA:1121:U:C6 | 2.43 | 0.54 |
| 1:QA:1315:U:H2' | 1:QA:1316:G:O4' | 2.07 | 0.54 |
| 1:QA:1371:G:O3' | 9:QI:69:GLY:HA3 | 2.08 | 0.54 |
| 2:QB:164:VAL:HG12 | 2:QB:166:ASP:H | 1.71 | 0.54 |
| 22:QW:4:G:H2' | 22:QW:5:G:C8 | 2.43 | 0.54 |
| 25:RA:2467:C:H5' | 55:R9:18:ARG:HH21 | 1.72 | 0.54 |
| 25:RA:2753:A:H1' | 55:R9:28:GLU:HB2 | 1.88 | 0.54 |
| 29:RF:53:THR:O | 29:RF:57:VAL:HG23 | 2.07 | 0.54 |
| 32:RI:9:LEU:HD11 | 32:RI:12:LEU:HD22 | 1.90 | 0.54 |
| 1:XA:1371:G:O3' | 9:XI:69:GLY:HA3 | 2.08 | 0.54 |
| 1:XA:636:U:H2' | 1:XA:637:G:C8 | 2.41 | 0.54 |
| 25:YA:2525:G:C4' | 55:Y9:28:GLU:HA | 2.36 | 0.54 |
| 25:YA:2741:A:C6 | 55:Y9:30:PRO:HG2 | 2.43 | 0.54 |
| 25:YA:1830:C:H2' | 25:YA:1831:G:H8 | 1.73 | 0.54 |
| 25:YA:2243:U:H2' | 25:YA:2244:U:C6 | 2.42 | 0.54 |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:C6 | 2.43 | 0.54 |
| 35:YP:68:GLN:HG2 | 54:Y8:12:LYS:HG2 | 1.89 | 0.54 |
| 1:QA:1432:G:O2' | 1:QA:1468:A:N6 | 2.41 | 0.54 |
| 13:QM:3:ARG:HH22 | 30:RG:113:ARG:HH21 | 1.56 | 0.54 |
| 48:R2:16:LEU:HD21 | 48:R2:20:GLU:HG3 | 1.90 | 0.54 |
| 25:RA:1246:A:OP1 | 35:RP:15:ARG:NH2 | 2.35 | 0.54 |
| 25:RA:1538:G:H2' | 25:RA:1539:G:H8 | 1.72 | 0.54 |
| 30:RG:80:PHE:HE2 | 30:RG:82:LEU:HD12 | 1.72 | 0.54 |
| 35:RP:135:LEU:HG | 35:RP:139:LYS:HE2 | 1.89 | 0.54 |
| 36:RQ:65:PHE:HB2 | 36:RQ:105:GLU:HB3 | 1.89 | 0.54 |
| 45:RZ:102:LEU:HD23 | 45:RZ:137:ILE:HB | 1.90 | 0.54 |
| 1:XA:1427:U:H2' | 1:XA:1428:A:C8 | 2.43 | 0.54 |
| 1:XA:991:U:O4 | 1:XA:1212:U:O2' | 2.19 | 0.54 |
| 6:XF:36:ARG:NH2 | 6:XF:66:GLU:OE1 | 2.41 | 0.54 |
| 1:XA:192:U:O2' | 20:XT:60:GLU:OE2 | 2.22 | 0.54 |
| 22:XW:4:G:H2' | 22:XW:5:G:H8 | 1.73 | 0.54 |
| 55:Y9:2:LYS:HD2 | 55:Y9:31:LYS:HG2 | 1.90 | 0.54 |
| 25:YA:184:C:H2' | 25:YA:185:U:C6 | 2.43 | 0.54 |
| 25:YA:2443:C:H2' | 25:YA:2444:G:H8 | 1.73 | 0.54 |
| 25:YA:2535:G:H2' | 25:YA:2536:G:C8 | 2.42 | 0.54 |
| 25:YA:2740:A:N6 | 25:YA:2764:A:C8 | 2.76 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2741:A:H3' | 55:Y9:30:PRO:C | 2.27 | 0.54 |
| 25:YA:2599:G:H8 | 27:YD:236:GLY:HA2 | 1.72 | 0.54 |
| 35:YP:61:ARG:HG3 | 54:Y8:13:ARG:HD3 | 1.89 | 0.54 |
| 45:YZ:70:LEU:HG | 45:YZ:91:LEU:HD21 | 1.90 | 0.54 |
| 1:QA:486:U:H2' | 1:QA:487:A:H8 | 1.72 | 0.54 |
| 1:QA:514:C:H2' | 1:QA:515:G:C8 | 2.43 | 0.54 |
| 5:QE:34:VAL:HG11 | 5:QE:63:ARG:HE | 1.72 | 0.54 |
| 25:RA:2753:A:O2' | 55:R9:28:GLU:O | 2.25 | 0.54 |
| 25:RA:65:C:H2' | 25:RA:66:C:H6 | 1.72 | 0.54 |
| 28:RE:170:LEU:HD21 | 28:RE:187:ALA:HB3 | 1.90 | 0.54 |
| 1:XA:312:C:H2' | 1:XA:313:A:C8 | 2.43 | 0.54 |
| 1:XA:662:G:H2' | 1:XA:663:A:C8 | 2.42 | 0.54 |
| 1:XA:918:A:H2' | 1:XA:919:A:C8 | 2.43 | 0.54 |
| 1:XA:707:C:H4' | 11:XK:20:TYR:HD2 | 1.73 | 0.54 |
| 43:YX:11:PRO:HD3 | 48:Y2:37:PHE:CD1 | 2.42 | 0.54 |
| 25:YA:1946:U:H2' | 25:YA:1947:C:C6 | 2.43 | 0.54 |
| 25:YA:2527:C:H1' | 55:Y9:12:ASP:O | 2.07 | 0.54 |
| 25:YA:2539:C:O2' | 25:YA:2741:A:O2' | 2.22 | 0.54 |
| 25:YA:2764:A:N6 | 25:YA:2766:G:N3 | 2.56 | 0.54 |
| 25:YA:2303:G:N3 | 30:YG:132:ASN:ND2 | 2.55 | 0.54 |
| 30:YG:40:ASN:ND2 | 30:YG:90:LEU:O | 2.41 | 0.54 |
| 36:YQ:24:GLY:HA2 | 36:YQ:67:ARG:HH21 | 1.73 | 0.54 |
| 37:YR:88:ARG:NH2 | 37:YR:89:ASP:OD1 | 2.41 | 0.54 |
| 1:QA:789:U:H1' | 1:QA:792:A:H2 | 1.72 | 0.54 |
| 4:QD:50:ARG:HD2 | 4:QD:51:PRO:HD2 | 1.90 | 0.54 |
| 32:RI:72:LEU:HD11 | 32:RI:101:LEU:HD11 | 1.89 | 0.54 |
| 36:RQ:24:GLY:HA2 | 36:RQ:67:ARG:HH21 | 1.73 | 0.54 |
| 1:XA:1469:G:H2' | 1:XA:1470:G:C8 | 2.43 | 0.54 |
| 25:YA:1186:G:H2' | 25:YA:1187:G:O4' | 2.08 | 0.54 |
| 25:YA:1510:A:O2' | 25:YA:1512:G:N7 | 2.40 | 0.54 |
| 25:YA:1796:U:H2' | 25:YA:1797:C:C6 | 2.43 | 0.54 |
| 25:YA:2126:A:N6 | 25:YA:2163:C:O2' | 2.28 | 0.54 |
| 25:YA:397:G:O2' | 25:YA:2230:G:N2 | 2.38 | 0.54 |
| 25:YA:2525:G:O2' | 25:YA:2526:G:H8 | 1.91 | 0.54 |
| 45:YZ:114:GLY:HA3 | 45:YZ:177:PRO:HG3 | 1.88 | 0.54 |
| 1:QA:707:C:H4' | 11:QK:20:TYR:HD2 | 1.73 | 0.54 |
| 15:QO:15:PHE:HD2 | 15:QO:30:ALA:HB2 | 1.73 | 0.54 |
| 25:RA:184:C:H2' | 25:RA:185:U:H6 | 1.73 | 0.54 |
| 25:RA:2805:G:H2' | 25:RA:2807:G:C8 | 2.42 | 0.54 |
| 25:RA:92:G:H2' | 25:RA:93:C:H6 | 1.73 | 0.54 |
| 28:RE:23:VAL:HG12 | 28:RE:173:VAL:HG21 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:2193:G:H2' | 25:YA:2194:G:H8 | 1.72 | 0.54 |
| 25:YA:2785:C:H2' | 25:YA:2786:U:C6 | 2.43 | 0.54 |
| 29:YF:53:THR:O | 29:YF:57:VAL:HG23 | 2.08 | 0.54 |
| 1:QA:1004:A:C2 | 1:QA:1025:U:H1' | 2.43 | 0.53 |
| 2:QB:19:HIS:CD2 | 2:QB:206:ASP:HB2 | 2.43 | 0.53 |
| 35:RP:64:LYS:HB2 | 54:R8:25:MET:HG3 | 1.90 | 0.53 |
| 25:RA:1166:C:H2' | 25:RA:1167:U:C6 | 2.42 | 0.53 |
| 25:RA:2567:G:H2' | 25:RA:2568:C:C6 | 2.44 | 0.53 |
| 25:RA:2688:U:OP1 | 25:RA:2713:A:N6 | 2.41 | 0.53 |
| 1:XA:1105:A:H2' | 1:XA:1106:G:H8 | 1.72 | 0.53 |
| 1:XA:1210:C:O2' | 1:XA:1213:A:O2' | 2.26 | 0.53 |
| 1:XA:316:G:OP2 | 1:XA:351:G:O2' | 2.16 | 0.53 |
| 1:XA:359:U:H2' | 1:XA:360:A:H8 | 1.72 | 0.53 |
| 9:XI:49:PRO:HB2 | 9:XI:85:LEU:HD21 | 1.90 | 0.53 |
| 25:YA:2526:G:H21 | 55:Y9:13:LYS:HZ3 | 1.53 | 0.53 |
| 25:YA:2755:C:C6 | 55:Y9:35:ARG:HB3 | 2.42 | 0.53 |
| 25:YA:1184:G:P | 49:Y3:29:ARG:HH12 | 2.31 | 0.53 |
| 25:YA:2311:A:C8 | 30:YG:82:LEU:HD11 | 2.43 | 0.53 |
| 25:YA:439:G:H2' | 25:YA:440:G:H8 | 1.73 | 0.53 |
| 25:YA:729:G:P | 27:YD:13:ARG:HD3 | 2.48 | 0.53 |
| 45:YZ:56:VAL:HG22 | 45:YZ:70:LEU:HD21 | 1.89 | 0.53 |
| 1:QA:1218:C:H2' | 1:QA:1219:U:H6 | 1.73 | 0.53 |
| 1:QA:946:A:O2' | 1:QA:1333:A:N3 | 2.35 | 0.53 |
| 2:QB:213:LEU:HD11 | 2:QB:217:ARG:HE | 1.73 | 0.53 |
| 25:RA:1417:C:H2' | 25:RA:1418:G:O4' | 2.08 | 0.53 |
| 25:RA:270(D):C:H2' | 25:RA:270(E):G:H8 | 1.74 | 0.53 |
| 25:RA:2627:G:O2' | 25:RA:2781:A:N1 | 2.34 | 0.53 |
| 25:RA:30:G:H2' | 25:RA:31:C:H6 | 1.73 | 0.53 |
| 43:RX:53:LYS:NZ | 43:RX:55:ASN:OD1 | 2.41 | 0.53 |
| 1:XA:17:U:H2' | 1:XA:18:C:H6 | 1.71 | 0.53 |
| 9:XI:47:LEU:HD12 | 9:XI:50:LEU:HD12 | 1.90 | 0.53 |
| 13:XM:15:VAL:HG22 | 13:XM:45:VAL:HB | 1.88 | 0.53 |
| 1:XA:974:A:H5'' | 14:YN:31:ARG:HD3 | 1.89 | 0.53 |
| 48:Y2:66:GLU:HG2 | 48:Y2:69:ARG:HH21 | 1.74 | 0.53 |
| 52:Y6:10:LEU:HD23 | 52:Y6:22:ALA:HB2 | 1.89 | 0.53 |
| 25:YA:30:G:O2' | 25:YA:1214:A:N3 | 2.33 | 0.53 |
| 25:YA:2315:G:H2' | 25:YA:2316:C:C6 | 2.43 | 0.53 |
| 29:YF:184:TYR:CE2 | 29:YF:188:ARG:HD2 | 2.43 | 0.53 |
| 25:YA:2749:A:OP1 | 31:YH:4:ILE:HG23 | 2.08 | 0.53 |
| 1:QA:269:C:H2' | 1:QA:270:A:H8 | 1.74 | 0.53 |
| 2:QB:61:LEU:HG | 2:QB:66:GLY:HA3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:513:A:O2' | 25:RA:1217:C:OP1 | 2.26 | 0.53 |
| 27:RD:44:ASN:HB2 | 27:RD:48:ARG:O | 2.08 | 0.53 |
| 28:RE:24:THR:OG1 | 28:RE:186:GLY:HA2 | 2.08 | 0.53 |
| 31:RH:69:ARG:NH1 | 31:RH:73:ALA:HB2 | 2.23 | 0.53 |
| 1:XA:1351:U:H3 | 1:XA:1371:G:H1 | 1.56 | 0.53 |
| 1:XA:700:G:H4' | 1:XA:704:A:H1' | 1.90 | 0.53 |
| 2:XB:130:ARG:NE | 2:XB:134:GLU:OE1 | 2.36 | 0.53 |
| 25:YA:2306:C:N4 | 30:YG:42:GLY:O | 2.42 | 0.53 |
| 39:YT:20:PRO:HD2 | 39:YT:86:ILE:HG23 | 1.89 | 0.53 |
| 1:QA:1095:U:OP1 | 1:QA:1108:G:N2 | 2.34 | 0.53 |
| 1:QA:272:C:H2' | 1:QA:273:A:H8 | 1.73 | 0.53 |
| 1:QA:356:A:N3 | 1:QA:368:U:O2' | 2.38 | 0.53 |
| 1:QA:422:C:O2' | 1:QA:423:G:N2 | 2.42 | 0.53 |
| 2:QB:178:ARG:NH2 | 2:QB:196:LEU:O | 2.40 | 0.53 |
| 9:QI:48:GLU:HB2 | 9:QI:78:LYS:HE3 | 1.89 | 0.53 |
| 25:RA:1020:A:N1 | 25:RA:1141:U:H2' | 2.23 | 0.53 |
| 25:RA:2146:C:H4' | 25:RA:2147:G:C8 | 2.44 | 0.53 |
| 25:RA:2197:U:H1' | 25:RA:2198:A:H8 | 1.74 | 0.53 |
| 25:RA:997:G:OP1 | 40:RU:93:LYS:HB2 | 2.08 | 0.53 |
| 30:RG:173:LEU:HD22 | 30:RG:178:PHE:CE2 | 2.43 | 0.53 |
| 37:RR:17:ARG:HG2 | 37:RR:21:TYR:CE2 | 2.44 | 0.53 |
| 1:XA:1244:C:H2' | 1:XA:1245:A:H8 | 1.72 | 0.53 |
| 1:XA:908:A:H2' | 1:XA:909:A:H8 | 1.73 | 0.53 |
| 25:YA:1048:A:OP2 | 25:YA:1110:G:N2 | 2.42 | 0.53 |
| 25:YA:1600:C:OP1 | 43:YX:58:HIS:NE2 | 2.23 | 0.53 |
| 25:YA:2032:G:OP2 | 25:YA:2454:G:O2' | 2.19 | 0.53 |
| 25:YA:2695:C:H2' | 25:YA:2696:U:C6 | 2.43 | 0.53 |
| 25:YA:2742:C:OP1 | 55:Y9:29:ASN:HB3 | 2.08 | 0.53 |
| 27:YD:52:ARG:NH1 | 27:YD:249:PRO:HG2 | 2.24 | 0.53 |
| 34:YO:102:VAL:HB | 34:YO:106:LEU:HD12 | 1.89 | 0.53 |
| 41:YV:55:ALA:HA | 41:YV:101:GLY:HA2 | 1.90 | 0.53 |
| 44:YY:8:LYS:HD3 | 44:YY:97:ARG:HH21 | 1.73 | 0.53 |
| 19:QS:10:PHE:CD1 | 19:QS:38:SER:HB2 | 2.43 | 0.53 |
| 19:QS:65:ASN:HA | 50:R4:58:ARG:HD2 | 1.90 | 0.53 |
| 25:RA:586:A:N1 | 25:RA:809:G:O2' | 2.37 | 0.53 |
| 25:RA:2674:G:H5'' | 34:RO:26:LYS:HE2 | 1.91 | 0.53 |
| 25:RA:1252:G:N2 | 40:RU:33:ARG:HB3 | 2.24 | 0.53 |
| 1:XA:1003:G:N2 | 1:XA:1005:A:H5' | 2.22 | 0.53 |
| 1:XA:824:C:H2' | 1:XA:825:G:C8 | 2.43 | 0.53 |
| 2:XB:174:VAL:HG13 | 2:XB:184:VAL:HG11 | 1.91 | 0.53 |
| 5:XE:42:GLY:HA3 | 5:XE:66:MET:HG2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1946:U:H2' | 25:YA:1947:C:H6 | 1.73 | 0.53 |
| 25:YA:2134:A:OP2 | 25:YA:2157:G:N2 | 2.41 | 0.53 |
| 25:YA:270(H):C:H2' | 25:YA:270(I):G:C8 | 2.44 | 0.53 |
| 25:YA:321:G:OP2 | 29:YF:135:LYS:HD3 | 2.09 | 0.53 |
| 25:YA:676:A:H8 | 25:YA:2070:G:H1' | 1.74 | 0.53 |
| 35:YP:115:LEU:HA | 35:YP:134:ALA:HB2 | 1.91 | 0.53 |
| 45:YZ:45:ASP:OD1 | 45:YZ:49:ARG:NE | 2.41 | 0.53 |
| 1:QA:1392:G:N2 | 1:QA:1502:A:H8 | 2.06 | 0.53 |
| 1:QA:19:C:H2' | 1:QA:20:U:C6 | 2.44 | 0.53 |
| 1:QA:501:C:H1' | 1:QA:549:C:H1' | 1.90 | 0.53 |
| 1:QA:5:U:O4 | 4:QD:87:GLY:N | 2.34 | 0.53 |
| 3:QC:130:VAL:HG21 | 3:QC:157:ILE:HG23 | 1.91 | 0.53 |
| 20:QT:69:GLY:O | 20:QT:73:HIS:HB2 | 2.07 | 0.53 |
| 25:RA:709:U:H2' | 25:RA:710:G:C8 | 2.44 | 0.53 |
| 30:RG:16:ARG:NH2 | 30:RG:28:VAL:O | 2.41 | 0.53 |
| 39:RT:28:VAL:HG23 | 39:RT:88:ILE:HA | 1.91 | 0.53 |
| 1:XA:343:U:O2 | 1:XA:346:G:N1 | 2.41 | 0.53 |
| 2:XB:118:LEU:HB3 | 2:XB:142:LEU:HD12 | 1.91 | 0.53 |
| 3:XC:138:VAL:HG13 | 3:XC:149:ALA:HB3 | 1.90 | 0.53 |
| 9:XI:125:TYR:HE2 | 9:XI:127:LYS:HE3 | 1.72 | 0.53 |
| 17:XQ:45:HIS:CD2 | 17:XQ:47:PRO:HG3 | 2.43 | 0.53 |
| 25:YA:2626:C:H2' | 25:YA:2627:G:C8 | 2.44 | 0.53 |
| 25:YA:2746:U:H5 | 55:Y9:35:ARG:NH1 | 2.05 | 0.53 |
| 27:YD:24:ILE:HD11 | 27:YD:91:ARG:HD2 | 1.89 | 0.53 |
| 25:RA:1184:G:P | 49:R3:29:ARG:HH12 | 2.31 | 0.53 |
| 25:RA:2375:G:N2 | 25:RA:2378:A:OP2 | 2.39 | 0.53 |
| 28:RE:36:ARG:HH12 | 28:RE:86:PRO:HD2 | 1.73 | 0.53 |
| 30:RG:107:LEU:HD21 | 30:RG:178:PHE:CD1 | 2.44 | 0.53 |
| 25:RA:1651:G:H5' | 37:RR:39:PRO:HG2 | 1.91 | 0.53 |
| 40:RU:90:VAL:HG22 | 41:RV:39:LEU:HB3 | 1.91 | 0.53 |
| 1:XA:1004:A:OP1 | 1:XA:1025:U:N3 | 2.42 | 0.53 |
| 1:XA:158:G:H2' | 1:XA:159:G:C8 | 2.44 | 0.53 |
| 1:XA:405:U:O4 | 4:XD:2:GLY:N | 2.42 | 0.53 |
| 20:XT:26:ASN:HA | 20:XT:29:LYS:HG2 | 1.90 | 0.53 |
| 22:XW:4:G:H2' | 22:XW:5:G:C8 | 2.43 | 0.53 |
| 25:YA:1689:A:H2' | 25:YA:1690:A:H8 | 1.73 | 0.53 |
| 25:YA:570:G:H1' | 25:YA:983:A:N6 | 2.24 | 0.53 |
| 25:YA:852:G:H2' | 25:YA:853:G:H8 | 1.72 | 0.53 |
| 29:YF:143:ALA:HB1 | 29:YF:148:LEU:HB2 | 1.90 | 0.53 |
| 42:YW:76:VAL:HG22 | 42:YW:103:ILE:HA | 1.91 | 0.53 |
| 1:QA:21:G:H2' | 1:QA:22:G:C8 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:674:G:H2' | 1:QA:675:A:C8 | 2.43 | 0.53 |
| 1:QA:838:G:C6 | 1:QA:842:C:H1' | 2.44 | 0.53 |
| 4:QD:98:GLU:HG2 | 4:QD:189:PRO:HG3 | 1.90 | 0.53 |
| 9:QI:8:GLY:HA2 | 9:QI:79:LEU:HD12 | 1.91 | 0.53 |
| 25:RA:1425:G:H2' | 25:RA:1426:G:C8 | 2.44 | 0.53 |
| 25:RA:2030:A:H4' | 25:RA:2031:A:C8 | 2.42 | 0.53 |
| 25:RA:38:A:H2' | 25:RA:39:C:H6 | 1.74 | 0.53 |
| 27:RD:132:PRO:HG3 | 27:RD:190:TYR:CE1 | 2.41 | 0.53 |
| 25:RA:2224:G:OP1 | 27:RD:268:ARG:NH1 | 2.39 | 0.53 |
| 1:XA:464:G:C6 | 1:XA:466:C:H5' | 2.44 | 0.53 |
| 3:XC:130:VAL:HG21 | 3:XC:157:ILE:HG23 | 1.90 | 0.53 |
| 6:XF:6:VAL:HB | 6:XF:63:TYR:HB2 | 1.91 | 0.53 |
| 11:XK:91:ARG:O | 11:XK:95:ILE:HG12 | 2.09 | 0.53 |
| 48:Y2:16:LEU:HD21 | 48:Y2:20:GLU:HG3 | 1.91 | 0.53 |
| 49:Y3:3:ARG:NH2 | 49:Y3:60:GLU:OXT | 2.42 | 0.53 |
| 25:YA:1108:U:H2' | 25:YA:1109:C:C6 | 2.42 | 0.53 |
| 25:YA:1568:G:P | 27:YD:63:ARG:HH22 | 2.32 | 0.53 |
| 25:YA:2099:U:H3 | 25:YA:2190:G:H1 | 1.54 | 0.53 |
| 25:YA:2648:C:H2' | 25:YA:2649:U:C6 | 2.44 | 0.53 |
| 25:YA:2848:G:O2' | 25:YA:2867:G:N2 | 2.39 | 0.53 |
| 25:YA:439:G:H2' | 25:YA:440:G:C8 | 2.44 | 0.53 |
| 28:YE:48:GLN:OE1 | 28:YE:64:LYS:NZ | 2.40 | 0.53 |
| 34:YO:25:LEU:HB2 | 34:YO:38:VAL:HG13 | 1.90 | 0.53 |
| 39:YT:77:PRO:HB2 | 39:YT:80:SER:HB2 | 1.89 | 0.53 |
| 36:YQ:137:TYR:HB3 | 45:YZ:76:LEU:HD11 | 1.91 | 0.53 |
| 1:QA:1522:U:H2' | 1:QA:1523:G:H8 | 1.74 | 0.53 |
| 1:QA:399:G:H2' | 1:QA:400:C:C6 | 2.43 | 0.53 |
| 1:QA:946:A:H2' | 1:QA:947:G:C8 | 2.43 | 0.53 |
| 2:QB:130:ARG:NE | 2:QB:134:GLU:OE1 | 2.42 | 0.53 |
| 3:QC:11:ARG:NH2 | 3:QC:175:LEU:O | 2.41 | 0.53 |
| 3:QC:9:GLY:HA2 | 3:QC:12:LEU:HG | 1.90 | 0.53 |
| 1:QA:49:U:H4' | 12:QL:28:LYS:NZ | 2.24 | 0.53 |
| 22:QW:1:C:H42 | 22:QW:73:A:H61 | 1.56 | 0.53 |
| 25:RA:1224:G:N2 | 25:RA:1227:A:OP2 | 2.34 | 0.53 |
| 25:RA:754:C:H2' | 25:RA:755:C:H6 | 1.74 | 0.53 |
| 25:RA:320:A:H2' | 29:RF:136:THR:HG21 | 1.90 | 0.53 |
| 1:XA:1060:C:H2' | 1:XA:1061:G:H8 | 1.74 | 0.53 |
| 2:XB:72:GLY:HA3 | 2:XB:81:VAL:HG21 | 1.91 | 0.53 |
| 1:XA:1286:A:H5'' | 21:XU:26:LYS:HD2 | 1.91 | 0.53 |
| 49:Y3:6:VAL:HB | 49:Y3:54:VAL:HG21 | 1.90 | 0.53 |
| 25:YA:806:C:O2 | 25:YA:2444:G:O2' | 2.26 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:2022:U:O2' | 25:YA:2617:C:H5' | 2.08 | 0.53 |
| 28:YE:36:ARG:HG3 | 28:YE:47:VAL:HG12 | 1.90 | 0.53 |
| 40:YU:91:ASP:O | 40:YU:93:LYS:N | 2.42 | 0.53 |
| 1:QA:254:G:O2' | 17:QQ:16:GLN:O | 2.27 | 0.53 |
| 25:RA:1085:A:O2' | 25:RA:1086:A:O5' | 2.27 | 0.53 |
| 25:RA:1336:A:H2' | 25:RA:1337:G:C8 | 2.43 | 0.53 |
| 25:RA:1882:C:H3' | 25:RA:1883:G:H8 | 1.73 | 0.53 |
| 27:RD:231:HIS:CD2 | 27:RD:249:PRO:HG3 | 2.44 | 0.53 |
| 1:XA:427:U:OP2 | 1:XA:428:G:O2' | 2.19 | 0.53 |
| 2:XB:42:ILE:HD11 | 2:XB:202:PRO:HB2 | 1.91 | 0.53 |
| 7:XG:15:ASP:OD1 | 7:XG:16:LEU:N | 2.42 | 0.53 |
| 55:Y9:21:GLY:O | 55:Y9:22:ARG:HD2 | 2.08 | 0.53 |
| 25:YA:1791:A:N6 | 25:YA:1828:G:O2' | 2.42 | 0.53 |
| 25:YA:2741:A:C5 | 55:Y9:30:PRO:HD2 | 2.44 | 0.53 |
| 25:YA:685:A:OP1 | 25:YA:686:G:N2 | 2.38 | 0.53 |
| 22:XV:57:C:N4 | 30:YG:83:ARG:HH12 | 2.06 | 0.53 |
| 1:QA:1068:G:OP1 | 1:QA:1387:G:O2' | 2.26 | 0.52 |
| 1:QA:1343:G:H2' | 1:QA:1344:C:C6 | 2.44 | 0.52 |
| 1:QA:736:C:H2' | 1:QA:737:A:H8 | 1.73 | 0.52 |
| 1:QA:973:G:O6 | 1:QA:974:A:N6 | 2.43 | 0.52 |
| 1:QA:1250:A:H4' | 9:QI:67:GLY:HA2 | 1.92 | 0.52 |
| 22:QW:8:U:O2 | 22:QW:14:A:N7 | 2.42 | 0.52 |
| 30:RG:179:PRO:HB3 | 50:R4:43:TYR:HE1 | 1.74 | 0.52 |
| 25:RA:1107:G:H2' | 25:RA:1108:U:C6 | 2.44 | 0.52 |
| 25:RA:2287:A:H62 | 25:RA:2344:U:H3 | 1.57 | 0.52 |
| 25:RA:270(Q):C:H5' | 32:RI:46:ALA:HB2 | 1.91 | 0.52 |
| 26:RB:24:G:O6 | 26:RB:56:G:O2' | 2.21 | 0.52 |
| 39:RT:77:PRO:HB2 | 39:RT:80:SER:HB2 | 1.91 | 0.52 |
| 1:XA:1121:U:H2' | 1:XA:1122:U:C6 | 2.44 | 0.52 |
| 1:XA:1510:U:H2' | 1:XA:1511:G:C8 | 2.44 | 0.52 |
| 1:XA:45:U:H2' | 1:XA:46:G:H8 | 1.74 | 0.52 |
| 30:YG:65:GLY:HA2 | 50:Y4:7:PRO:HG2 | 1.91 | 0.52 |
| 25:YA:2741:A:C2 | 55:Y9:30:PRO:HD2 | 2.43 | 0.52 |
| 25:YA:1641:A:H2' | 25:YA:1642:G:O4' | 2.09 | 0.52 |
| 25:YA:1991:U:H2' | 25:YA:1992:G:H5'' | 1.90 | 0.52 |
| 25:YA:2010:G:H5'' | 42:YW:42:ARG:HB2 | 1.91 | 0.52 |
| 31:YH:107:VAL:HB | 31:YH:153:LYS:NZ | 2.23 | 0.52 |
| 32:YI:78:THR:HG22 | 32:YI:141:LYS:HE3 | 1.91 | 0.52 |
| 42:YW:24:ILE:HD13 | 42:YW:36:LEU:HD11 | 1.90 | 0.52 |
| 45:YZ:54:HIS:HB3 | 45:YZ:101:PRO:HD3 | 1.91 | 0.52 |
| 1:QA:1151:A:H2' | 1:QA:1152:A:C8 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:407:G:H2' | 1:QA:408:A:C8 | 2.44 | 0.52 |
| 3:QC:19:GLU:HG2 | 3:QC:54:ARG:HE | 1.74 | 0.52 |
| 11:QK:57:THR:HG22 | 11:QK:59:TYR:H | 1.74 | 0.52 |
| 46:R0:32:ARG:N | 46:R0:35:ASN:OD1 | 2.42 | 0.52 |
| 25:RA:512:G:H4' | 25:RA:513:A:O5' | 2.08 | 0.52 |
| 37:RR:21:TYR:HE1 | 37:RR:43:GLU:HB3 | 1.74 | 0.52 |
| 1:XA:662:G:O2' | 1:XA:836:G:OP1 | 2.28 | 0.52 |
| 25:YA:2185:C:H2' | 25:YA:2186:G:C8 | 2.41 | 0.52 |
| 25:YA:2543:G:H2' | 25:YA:2544:G:C8 | 2.44 | 0.52 |
| 27:YD:36:PRO:CB | 27:YD:61:LEU:HB3 | 2.39 | 0.52 |
| 28:YE:37:ARG:HD3 | 28:YE:42:ASP:OD2 | 2.09 | 0.52 |
| 30:YG:19:LEU:HD11 | 30:YG:172:LEU:HD13 | 1.91 | 0.52 |
| 34:YO:104:ARG:NH1 | 34:YO:121:VAL:O | 2.42 | 0.52 |
| 1:QA:662:G:H2' | 1:QA:663:A:C8 | 2.45 | 0.52 |
| 25:RA:1000:A:H2' | 25:RA:1001:A:C8 | 2.44 | 0.52 |
| 31:RH:130:ARG:NH1 | 31:RH:132:ARG:HE | 2.06 | 0.52 |
| 32:RI:30:LEU:HB3 | 32:RI:36:ALA:HB3 | 1.91 | 0.52 |
| 36:RQ:31:ASP:OD1 | 36:RQ:134:ARG:NH1 | 2.43 | 0.52 |
| 1:XA:828:A:N3 | 2:XB:26:PRO:HG2 | 2.24 | 0.52 |
| 22:XW:8:U:O2 | 22:XW:14:A:N7 | 2.43 | 0.52 |
| 25:YA:2744:G:OP1 | 55:Y9:19:ARG:HB2 | 2.10 | 0.52 |
| 25:YA:2755:C:O4' | 55:Y9:35:ARG:NH1 | 2.41 | 0.52 |
| 25:YA:2355:C:H1' | 46:Y0:39:ARG:HH21 | 1.75 | 0.52 |
| 25:YA:2787:C:H1' | 28:YE:62:PRO:HG3 | 1.91 | 0.52 |
| 25:YA:665:C:H2' | 25:YA:666:G:H8 | 1.75 | 0.52 |
| 29:YF:107:LYS:HB3 | 29:YF:206:ILE:HD12 | 1.91 | 0.52 |
| 29:YF:78:ILE:HA | 29:YF:83:PHE:CD2 | 2.45 | 0.52 |
| 30:YG:121:ASN:HA | 30:YG:181:ARG:HH21 | 1.74 | 0.52 |
| 32:YI:9:LEU:HD11 | 32:YI:12:LEU:HD22 | 1.90 | 0.52 |
| 4:QD:15:GLU:OE2 | 4:QD:59:ARG:NH1 | 2.42 | 0.52 |
| 50:R4:28:LYS:HB2 | 50:R4:31:ILE:HD11 | 1.91 | 0.52 |
| 25:RA:1028:A:H2' | 25:RA:1029:A:C8 | 2.44 | 0.52 |
| 25:RA:1124:C:H2' | 25:RA:1125:G:O4' | 2.09 | 0.52 |
| 25:RA:1839:G:C2 | 25:RA:1840:G:C8 | 2.97 | 0.52 |
| 25:RA:2477:C:O2 | 55:R9:36:GLN:NE2 | 2.42 | 0.52 |
| 25:RA:2051:A:H5' | 25:RA:2578:G:O4' | 2.10 | 0.52 |
| 25:RA:2597:G:H5' | 27:RD:243:GLY:HA3 | 1.91 | 0.52 |
| 25:RA:2832:U:H4' | 25:RA:2833:G:H5'' | 1.92 | 0.52 |
| 27:RD:43:ARG:NH1 | 27:RD:49:ILE:HB | 2.24 | 0.52 |
| 33:RN:12:ARG:HH11 | 33:RN:14:VAL:HG22 | 1.74 | 0.52 |
| 1:XA:89:U:O2' | 1:XA:90:C:OP1 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:XB:16:HIS:HD2 | 2:XB:210:SER:HA | 1.74 | 0.52 |
| 9:XI:19:LEU:HD23 | 9:XI:61:ALA:HB2 | 1.91 | 0.52 |
| 25:YA:2743:C:C3' | 55:Y9:25:VAL:HA | 2.39 | 0.52 |
| 25:YA:2291:U:H2' | 25:YA:2292:C:H6 | 1.75 | 0.52 |
| 25:YA:2492:U:H2' | 25:YA:2493:U:C6 | 2.44 | 0.52 |
| 25:YA:793:A:OP2 | 25:YA:2071:A:O2' | 2.26 | 0.52 |
| 34:YO:78:ARG:HH21 | 39:YT:103:ARG:NH2 | 2.08 | 0.52 |
| 39:YT:24:PRO:HA | 39:YT:49:VAL:HG13 | 1.91 | 0.52 |
| 1:QA:279:A:OP2 | 17:QQ:95:TYR:OH | 2.19 | 0.52 |
| 8:QH:112:LEU:HD23 | 8:QH:133:LEU:HA | 1.91 | 0.52 |
| 25:RA:1292:U:H2' | 25:RA:1293:C:H6 | 1.74 | 0.52 |
| 25:RA:1941:C:N4 | 25:RA:1965:C:O4' | 2.42 | 0.52 |
| 25:RA:226:G:N2 | 25:RA:230:U:O4 | 2.43 | 0.52 |
| 1:XA:574:A:N3 | 1:XA:883:C:H1' | 2.23 | 0.52 |
| 6:XF:44:GLY:HA2 | 6:XF:59:TYR:CE1 | 2.45 | 0.52 |
| 25:YA:127:A:H5'' | 25:YA:128:C:C6 | 2.44 | 0.52 |
| 25:YA:1754:C:OP1 | 39:YT:96:ARG:NH1 | 2.42 | 0.52 |
| 25:YA:1889:A:N3 | 25:YA:2086:U:O2' | 2.40 | 0.52 |
| 1:QA:1213:A:N6 | 1:QA:1215:G:N3 | 2.58 | 0.52 |
| 1:QA:186(C):G:H1 | 1:QA:191(D):U:H3 | 1.57 | 0.52 |
| 1:QA:243:A:H4' | 1:QA:244:U:O5' | 2.09 | 0.52 |
| 1:QA:824:C:H2' | 1:QA:825:G:H8 | 1.74 | 0.52 |
| 17:QQ:51:TYR:CE2 | 17:QQ:73:VAL:HG11 | 2.44 | 0.52 |
| 22:QV:29:C:H2' | 22:QV:30:G:H8 | 1.74 | 0.52 |
| 25:RA:1416:G:H2' | 25:RA:1417:C:C6 | 2.45 | 0.52 |
| 25:RA:1996:C:OP1 | 34:RO:31:LYS:NZ | 2.43 | 0.52 |
| 25:RA:2306:C:H2' | 25:RA:2307:G:N2 | 2.24 | 0.52 |
| 25:RA:458:G:O2' | 25:RA:469:G:O6 | 2.26 | 0.52 |
| 26:RB:28:C:H2' | 26:RB:29:A:C8 | 2.44 | 0.52 |
| 43:RX:35:THR:HG23 | 43:RX:38:GLU:H | 1.73 | 0.52 |
| 1:XA:1314:C:H2' | 1:XA:1315:U:C6 | 2.45 | 0.52 |
| 1:XA:209:U:H1' | 1:XA:216:G:C6 | 2.45 | 0.52 |
| 1:XA:272:C:H2' | 1:XA:273:A:H8 | 1.73 | 0.52 |
| 13:XM:80:ARG:HD2 | 50:Y4:58:ARG:HD3 | 1.92 | 0.52 |
| 25:YA:2742:C:O2' | 55:Y9:25:VAL:HB | 2.10 | 0.52 |
| 25:YA:2154:G:H2' | 25:YA:2155:G:H8 | 1.74 | 0.52 |
| 25:YA:2742:C:P | 55:Y9:29:ASN:HB3 | 2.49 | 0.52 |
| 25:YA:2744:G:OP2 | 55:Y9:17:ILE:HG13 | 2.09 | 0.52 |
| 25:YA:2755:C:O2' | 25:YA:2756:U:H5 | 1.92 | 0.52 |
| 25:YA:997:G:OP1 | 40:YU:93:LYS:HB2 | 2.10 | 0.52 |
| 40:YU:97:ASP:OD1 | 40:YU:101:ARG:NH1 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1412:C:H2' | 1:QA:1413:A:C8 | 2.45 | 0.52 |
| 1:QA:563:A:H2' | 1:QA:567:G:H8 | 1.74 | 0.52 |
| 22:QW:5:G:H2' | 22:QW:6:G:H8 | 1.75 | 0.52 |
| 25:RA:1292:U:H2' | 25:RA:1293:C:C6 | 2.45 | 0.52 |
| 25:RA:185:U:C2 | 25:RA:212:G:N2 | 2.78 | 0.52 |
| 25:RA:2183:C:H2' | 25:RA:2184:G:H8 | 1.74 | 0.52 |
| 27:RD:108:PRO:HB3 | 27:RD:143:HIS:CE1 | 2.44 | 0.52 |
| 41:RV:62:LEU:HD11 | 41:RV:95:LEU:HB2 | 1.91 | 0.52 |
| 1:XA:922:G:H2' | 1:XA:923:A:C8 | 2.44 | 0.52 |
| 3:XC:58:GLU:HB2 | 3:XC:65:ALA:HB3 | 1.91 | 0.52 |
| 49:Y3:8:LEU:HG | 49:Y3:28:LEU:HD13 | 1.91 | 0.52 |
| 25:YA:458:G:H22 | 25:YA:469:G:H3' | 1.75 | 0.52 |
| 25:YA:807:U:H2' | 25:YA:808:G:H8 | 1.74 | 0.52 |
| 33:YN:73:THR:HB | 33:YN:82:LEU:HD11 | 1.92 | 0.52 |
| 1:QA:537:G:H5'' | 12:QL:113:ARG:NH1 | 2.24 | 0.52 |
| 25:RA:849:A:N1 | 49:R3:25:ALA:HB2 | 2.24 | 0.52 |
| 25:RA:1636:C:H2' | 25:RA:1637:A:H8 | 1.73 | 0.52 |
| 25:RA:2183:C:H2' | 25:RA:2184:G:C8 | 2.45 | 0.52 |
| 25:RA:2331:G:O2' | 46:R0:43:THR:HG22 | 2.09 | 0.52 |
| 25:RA:777:A:H2' | 25:RA:778:G:H8 | 1.75 | 0.52 |
| 25:RA:1818:U:H2' | 27:RD:157:ARG:HG2 | 1.91 | 0.52 |
| 27:RD:264:LYS:HE2 | 27:RD:266:SER:HB3 | 1.92 | 0.52 |
| 34:RO:3:GLN:HB2 | 34:RO:4:PRO:HD2 | 1.91 | 0.52 |
| 36:RQ:116:GLU:OE2 | 36:RQ:119:ARG:NH2 | 2.33 | 0.52 |
| 36:RQ:77:LYS:NZ | 36:RQ:84:GLY:O | 2.37 | 0.52 |
| 39:RT:123:GLN:O | 39:RT:125:ARG:N | 2.42 | 0.52 |
| 42:RW:11:ARG:HH21 | 42:RW:98:LYS:HD3 | 1.75 | 0.52 |
| 1:XA:753:A:H4' | 1:XA:754:C:O5' | 2.10 | 0.52 |
| 12:XL:60:LEU:HD12 | 12:XL:62:SER:H | 1.74 | 0.52 |
| 14:YN:24:CYS:HB3 | 14:YN:29:ARG:H | 1.74 | 0.52 |
| 35:YP:121:LYS:HD3 | 35:YP:122:PRO:HD2 | 1.91 | 0.52 |
| 1:QA:1251:A:H2' | 1:QA:1252:A:C8 | 2.45 | 0.52 |
| 1:QA:1317:C:H2' | 1:QA:1318:A:O4' | 2.10 | 0.52 |
| 1:QA:1513:A:H2' | 1:QA:1514:C:C6 | 2.45 | 0.52 |
| 1:QA:688:G:H2' | 1:QA:689:C:H6 | 1.74 | 0.52 |
| 1:QA:677:U:H3 | 1:QA:713:G:H22 | 1.58 | 0.52 |
| 1:QA:22:G:H4' | 1:QA:885:G:C8 | 2.45 | 0.52 |
| 12:QL:85:ILE:HG23 | 12:QL:98:TYR:HB3 | 1.91 | 0.52 |
| 54:R8:26:LYS:HD3 | 54:R8:47:LYS:HB3 | 1.91 | 0.52 |
| 25:RA:2074:U:H2' | 25:RA:2075:U:C6 | 2.45 | 0.52 |
| 38:RS:34:HIS:CD2 | 38:RS:54:LEU:HD12 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:RT:50:ILE:HG13 | 39:RT:99:LEU:HD12 | 1.91 | 0.52 |
| 25:RA:533:G:N2 | 40:RU:49:HIS:HE1 | 2.08 | 0.52 |
| 1:XA:980:C:H5'' | 1:XA:981:U:C5 | 2.45 | 0.52 |
| 22:XV:15:G:H1 | 22:XV:49:C:H5 | 1.56 | 0.52 |
| 25:YA:1935:G:H1' | 25:YA:1964:G:N2 | 2.24 | 0.52 |
| 25:YA:1990:C:H2' | 25:YA:1991:U:C6 | 2.45 | 0.52 |
| 26:YB:44:G:H1' | 26:YB:47:C:N4 | 2.25 | 0.52 |
| 27:YD:52:ARG:HH21 | 27:YD:53:PHE:HE2 | 1.57 | 0.52 |
| 26:YB:114:G:HO2' | 38:YS:50:SER:HG | 1.53 | 0.52 |
| 18:QR:31:LEU:HD23 | 18:QR:31:LEU:H | 1.75 | 0.52 |
| 47:R1:86:SER:N | 47:R1:87:PRO:HD2 | 2.25 | 0.52 |
| 52:R6:10:LEU:HG | 52:R6:54:ILE:HG13 | 1.92 | 0.52 |
| 35:RP:59:LEU:O | 54:R8:13:ARG:NH1 | 2.43 | 0.52 |
| 25:RA:1508:A:O2' | 25:RA:1509:C:O4' | 2.23 | 0.52 |
| 25:RA:2696:U:H2' | 25:RA:2697:G:C8 | 2.45 | 0.52 |
| 25:RA:689:A:H2' | 25:RA:690:G:C8 | 2.45 | 0.52 |
| 25:RA:793:A:OP2 | 25:RA:2071:A:O2' | 2.25 | 0.52 |
| 27:RD:72:LYS:HG3 | 27:RD:97:TYR:CE2 | 2.45 | 0.52 |
| 29:RF:124:LEU:HB3 | 29:RF:193:VAL:HG22 | 1.92 | 0.52 |
| 34:RO:102:VAL:HB | 34:RO:106:LEU:HD12 | 1.91 | 0.52 |
| 1:XA:1241:G:H1 | 1:XA:1296:C:H42 | 1.58 | 0.52 |
| 5:XE:97:GLY:N | 5:XE:117:ASP:OD2 | 2.40 | 0.52 |
| 22:XV:53:G:O2' | 22:XV:54:G:OP1 | 2.27 | 0.52 |
| 25:YA:2074:U:H2' | 25:YA:2075:U:C6 | 2.45 | 0.52 |
| 28:YE:104:VAL:HG22 | 28:YE:198:VAL:HG22 | 1.92 | 0.52 |
| 25:YA:807:U:OP2 | 35:YP:41:ARG:NH1 | 2.43 | 0.52 |
| 45:YZ:144:LEU:HD11 | 45:YZ:149:SER:HA | 1.91 | 0.52 |
| 3:QC:189:ALA:HB3 | 3:QC:196:LEU:H | 1.76 | 0.51 |
| 12:QL:35:GLY:HA2 | 12:QL:60:LEU:HA | 1.92 | 0.51 |
| 16:QP:3:LYS:HG3 | 16:QP:65:GLN:O | 2.10 | 0.51 |
| 20:QT:81:LYS:O | 20:QT:85:MET:HG2 | 2.10 | 0.51 |
| 25:RA:1050:A:H2' | 25:RA:1051:G:O4' | 2.10 | 0.51 |
| 25:RA:2065:C:H2' | 25:RA:2066:C:H6 | 1.74 | 0.51 |
| 25:RA:2126:A:H4' | 25:RA:2127:G:O5' | 2.10 | 0.51 |
| 25:RA:2600:A:H2' | 25:RA:2601:C:C6 | 2.45 | 0.51 |
| 31:RH:151:ILE:HG22 | 31:RH:153:LYS:HG2 | 1.92 | 0.51 |
| 31:RH:83:TYR:CE2 | 31:RH:138:LYS:HD2 | 2.46 | 0.51 |
| 43:RX:55:ASN:HB2 | 43:RX:80:ILE:HG23 | 1.91 | 0.51 |
| 1:XA:407:G:H2' | 1:XA:408:A:C8 | 2.44 | 0.51 |
| 22:XW:11:A:H2' | 22:XW:12:G:C8 | 2.45 | 0.51 |
| 25:YA:2836:U:H2' | 25:YA:2837:G:C8 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:YG:107:LEU:HD21 | 30:YG:178:PHE:CD1 | 2.45 | 0.51 |
| 32:YI:144:VAL:HG22 | 32:YI:145:VAL:H | 1.75 | 0.51 |
| 39:YT:24:PRO:HG3 | 39:YT:52:ILE:HD12 | 1.93 | 0.51 |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:H | 1.74 | 0.51 |
| 1:QA:1321:C:O2' | 19:QS:78:ARG:NH2 | 2.43 | 0.51 |
| 1:QA:403:C:H2' | 1:QA:404:U:H6 | 1.75 | 0.51 |
| 1:QA:484:G:H4' | 1:QA:485:G:O5' | 2.11 | 0.51 |
| 5:QE:107:ARG:O | 5:QE:111:GLU:HB2 | 2.09 | 0.51 |
| 9:QI:5:TYR:HE1 | 9:QI:16:ARG:HB2 | 1.74 | 0.51 |
| 1:QA:376:G:H5'' | 16:QP:5:ARG:HB2 | 1.91 | 0.51 |
| 24:QY:27:A:H2' | 24:QY:28:G:H8 | 1.75 | 0.51 |
| 25:RA:2262:U:H2' | 25:RA:2263:C:H6 | 1.76 | 0.51 |
| 25:RA:37:C:H2' | 25:RA:38:A:H8 | 1.74 | 0.51 |
| 36:RQ:39:PRO:HB3 | 36:RQ:99:PRO:HD3 | 1.92 | 0.51 |
| 1:XA:188:U:H2' | 1:XA:189:U:H5'' | 1.92 | 0.51 |
| 1:XA:345:C:H4' | 1:XA:346:G:O5' | 2.09 | 0.51 |
| 20:XT:69:GLY:O | 20:XT:73:HIS:HB2 | 2.10 | 0.51 |
| 25:YA:2248:C:H2' | 25:YA:2249:U:O4' | 2.11 | 0.51 |
| 25:YA:2564:A:N7 | 25:YA:2647:U:O2' | 2.43 | 0.51 |
| 25:YA:2741:A:H8 | 25:YA:2741:A:O5' | 1.94 | 0.51 |
| 25:YA:2744:G:C5' | 55:Y9:24:TYR:HB2 | 2.38 | 0.51 |
| 28:YE:23:VAL:HG21 | 28:YE:183:LEU:HD23 | 1.91 | 0.51 |
| 41:YV:62:LEU:HD11 | 41:YV:95:LEU:HB2 | 1.92 | 0.51 |
| 1:QA:110:C:O2' | 16:QP:25:ARG:O | 2.28 | 0.51 |
| 1:QA:1194:U:H4' | 5:QE:22:GLY:O | 2.10 | 0.51 |
| 2:QB:52:GLU:O | 2:QB:56:ARG:HG2 | 2.10 | 0.51 |
| 25:RA:177:G:H3' | 25:RA:178:G:H8 | 1.76 | 0.51 |
| 30:RG:63:ILE:HG22 | 30:RG:143:GLU:HB2 | 1.92 | 0.51 |
| 40:RU:95:LEU:HD13 | 41:RV:4:ILE:HD12 | 1.92 | 0.51 |
| 44:RY:35:TYR:CE2 | 44:RY:69:ALA:HB3 | 2.45 | 0.51 |
| 1:XA:392:G:HO2' | 1:XA:483:C:HO2' | 1.45 | 0.51 |
| 1:XA:606:G:H22 | 1:XA:631:G:H5'' | 1.75 | 0.51 |
| 1:XA:1108:G:H5' | 3:XC:176:HIS:CD2 | 2.46 | 0.51 |
| 10:XJ:50:ILE:HD13 | 10:XJ:60:ARG:HE | 1.75 | 0.51 |
| 25:YA:2354:G:H4' | 46:Y0:35:ASN:HD22 | 1.74 | 0.51 |
| 25:YA:1427:A:H4' | 25:YA:1428:C:O5' | 2.10 | 0.51 |
| 25:YA:2776:A:H4' | 25:YA:2777:G:O5' | 2.10 | 0.51 |
| 31:YH:149:ARG:NH2 | 55:Y9:18:ARG:HG2 | 2.26 | 0.51 |
| 1:QA:768:A:H5' | 1:QA:1524:C:H1' | 1.93 | 0.51 |
| 4:QD:119:GLN:CB | 4:QD:119:GLN:OE1 | 2.58 | 0.51 |
| 9:QI:113:LYS:H | 9:QI:119:ALA:HA | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1204:A:H1' | 25:RA:1206:G:C8 | 2.45 | 0.51 |
| 25:RA:1525:G:H2' | 25:RA:1526:G:C8 | 2.46 | 0.51 |
| 25:RA:1907:G:O6 | 25:RA:1924:C:N4 | 2.44 | 0.51 |
| 25:RA:2102:U:H2' | 25:RA:2103:C:C6 | 2.45 | 0.51 |
| 45:RZ:56:VAL:HG22 | 45:RZ:70:LEU:HD21 | 1.92 | 0.51 |
| 30:YG:105:LYS:HD3 | 50:Y4:26:SER:HB2 | 1.91 | 0.51 |
| 55:Y9:27:CYS:HB3 | 55:Y9:28:GLU:OE1 | 2.11 | 0.51 |
| 25:YA:2527:C:H2' | 25:YA:2528:U:O4' | 2.11 | 0.51 |
| 25:YA:270(S):G:H2' | 25:YA:270(T):G:H8 | 1.76 | 0.51 |
| 25:YA:2744:G:O2' | 31:YH:146:ALA:HB1 | 2.11 | 0.51 |
| 25:YA:783:A:H8 | 25:YA:784:A:H4' | 1.75 | 0.51 |
| 31:YH:152:ARG:HA | 55:Y9:19:ARG:HE | 1.76 | 0.51 |
| 33:YN:89:LYS:O | 33:YN:93:THR:HG22 | 2.10 | 0.51 |
| 13:QM:108:ARG:HE | 13:QM:114:ARG:HD2 | 1.75 | 0.51 |
| 19:QS:3:ARG:NE | 19:QS:7:LYS:HE2 | 2.19 | 0.51 |
| 25:RA:1198:U:H2' | 25:RA:1199:U:C6 | 2.45 | 0.51 |
| 25:RA:1310:G:OP2 | 53:R7:9:ARG:NE | 2.36 | 0.51 |
| 25:RA:1990:C:H2' | 25:RA:1991:U:C6 | 2.45 | 0.51 |
| 25:RA:297:C:H2' | 25:RA:298:G:O4' | 2.10 | 0.51 |
| 25:RA:796:C:H2' | 25:RA:797:C:C6 | 2.46 | 0.51 |
| 1:XA:1321:C:H5'' | 1:XA:1322:C:H5'' | 1.91 | 0.51 |
| 1:XA:414:A:OP2 | 1:XA:428:G:N2 | 2.43 | 0.51 |
| 1:XA:5:U:O2' | 1:XA:6:G:O5' | 2.28 | 0.51 |
| 1:XA:898:G:N2 | 1:XA:901:A:OP2 | 2.43 | 0.51 |
| 1:XA:1192:C:P | 3:XC:4:LYS:HZ1 | 2.33 | 0.51 |
| 7:XG:69:VAL:HG21 | 7:XG:104:LEU:HD21 | 1.93 | 0.51 |
| 24:XY:27:A:H2' | 24:XY:28:G:H8 | 1.74 | 0.51 |
| 25:YA:2102:U:H2' | 25:YA:2103:C:C6 | 2.45 | 0.51 |
| 25:YA:2421:G:N7 | 54:Y8:31:HIS:NE2 | 2.59 | 0.51 |
| 27:YD:244:ARG:HB2 | 27:YD:245:PRO:HD2 | 1.93 | 0.51 |
| 25:YA:1424:G:P | 27:YD:33:LEU:HD12 | 2.51 | 0.51 |
| 25:YA:39:C:O2 | 29:YF:46:ARG:NH2 | 2.43 | 0.51 |
| 39:YT:53:ARG:O | 39:YT:59:THR:HG23 | 2.11 | 0.51 |
| 39:YT:28:VAL:HG23 | 39:YT:88:ILE:HA | 1.93 | 0.51 |
| 1:QA:1128:C:H1' | 1:QA:1146:A:H61 | 1.75 | 0.51 |
| 1:QA:398:C:H2' | 1:QA:399:G:H8 | 1.76 | 0.51 |
| 1:QA:684:A:H1' | 11:QK:39:PRO:HD2 | 1.92 | 0.51 |
| 22:QW:4:G:H2' | 22:QW:5:G:H8 | 1.74 | 0.51 |
| 25:RA:1113:U:H2' | 25:RA:1114:G:C8 | 2.46 | 0.51 |
| 25:RA:2285:C:OP1 | 52:R6:29:ASN:ND2 | 2.44 | 0.51 |
| 25:RA:2314:C:H2' | 25:RA:2315:G:H8 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:638:G:H2' | 25:RA:639:U:C6 | 2.46 | 0.51 |
| 29:RF:34:TRP:CE3 | 35:RP:8:PRO:HB3 | 2.46 | 0.51 |
| 1:XA:1299:A:H2' | 1:XA:1301:U:H1' | 1.93 | 0.51 |
| 1:XA:1431:C:H2' | 1:XA:1432:G:O4' | 2.11 | 0.51 |
| 50:Y4:56:VAL:CG2 | 50:Y4:58:ARG:HG3 | 2.40 | 0.51 |
| 25:YA:1045:A:O2' | 25:YA:1046:A:OP2 | 2.24 | 0.51 |
| 25:YA:1844:C:H2' | 25:YA:1845:G:H8 | 1.74 | 0.51 |
| 25:YA:2627:G:O2' | 25:YA:2781:A:N1 | 2.37 | 0.51 |
| 25:YA:38:A:H2' | 25:YA:39:C:C6 | 2.46 | 0.51 |
| 31:YH:8:PRO:HG2 | 31:YH:69:ARG:NE | 2.17 | 0.51 |
| 40:YU:90:VAL:HG12 | 40:YU:91:ASP:H | 1.74 | 0.51 |
| 1:QA:1438:G:OP2 | 20:QT:34:LYS:NZ | 2.36 | 0.51 |
| 1:QA:188:U:H2' | 1:QA:189:U:H5'' | 1.93 | 0.51 |
| 1:QA:790:A:OP1 | 22:QV:39:A:O2' | 2.26 | 0.51 |
| 8:QH:110:ALA:HB3 | 8:QH:121:ASP:HB3 | 1.93 | 0.51 |
| 25:RA:2610:C:H4' | 25:RA:2611:U:OP2 | 2.11 | 0.51 |
| 45:RZ:70:LEU:HG | 45:RZ:91:LEU:HD21 | 1.92 | 0.51 |
| 1:XA:477:G:H2' | 1:XA:478:A:C8 | 2.46 | 0.51 |
| 25:YA:2093:G:H2' | 25:YA:2094:G:H8 | 1.75 | 0.51 |
| 25:YA:2308:G:H22 | 25:YA:2311:A:H2 | 1.58 | 0.51 |
| 32:YI:100:ALA:O | 32:YI:104:GLN:HB3 | 2.10 | 0.51 |
| 35:YP:97:PRO:O | 35:YP:98:GLU:HG2 | 2.11 | 0.51 |
| 38:YS:26:LEU:HB3 | 38:YS:87:PHE:HA | 1.92 | 0.51 |
| 1:QA:620:C:H4' | 4:QD:138:TYR:HD1 | 1.76 | 0.51 |
| 1:QA:908:A:H2' | 1:QA:909:A:H8 | 1.76 | 0.51 |
| 1:QA:976:G:OP1 | 14:QN:32:SER:N | 2.43 | 0.51 |
| 25:RA:1468:C:H2' | 25:RA:1469:A:C8 | 2.46 | 0.51 |
| 25:RA:1885:A:H5' | 25:RA:1886:C:OP2 | 2.11 | 0.51 |
| 25:RA:2637:U:H5'' | 28:RE:82:ARG:NH1 | 2.25 | 0.51 |
| 25:RA:270(S):G:H2' | 25:RA:270(T):G:H8 | 1.76 | 0.51 |
| 27:RD:242:ARG:O | 27:RD:244:ARG:HG2 | 2.11 | 0.51 |
| 30:RG:32:PRO:HB2 | 30:RG:172:LEU:HD22 | 1.91 | 0.51 |
| 33:RN:89:LYS:O | 33:RN:93:THR:HG22 | 2.11 | 0.51 |
| 15:XO:7:GLU:OE2 | 15:XO:38:ARG:NH2 | 2.44 | 0.51 |
| 28:YE:52:LEU:HB2 | 28:YE:75:VAL:HB | 1.93 | 0.51 |
| 31:YH:137:ASP:OD1 | 31:YH:138:LYS:N | 2.38 | 0.51 |
| 44:YY:35:TYR:CE2 | 44:YY:69:ALA:HB3 | 2.46 | 0.51 |
| 1:QA:1120:G:H2' | 1:QA:1121:U:H6 | 1.75 | 0.51 |
| 5:QE:97:GLY:N | 5:QE:117:ASP:OD2 | 2.38 | 0.51 |
| 10:QJ:23:ILE:HG23 | 10:QJ:85:LEU:HD22 | 1.92 | 0.51 |
| 25:RA:2646:C:OP2 | 25:RA:2732:G:O2' | 2.15 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2892:A:H2' | 25:RA:2893:G:O4' | 2.10 | 0.51 |
| 25:RA:530:G:C6 | 25:RA:2022:U:H5'' | 2.46 | 0.51 |
| 25:RA:792:G:N3 | 25:RA:2072:G:O2' | 2.40 | 0.51 |
| 26:RB:29:A:H2' | 26:RB:30:C:C6 | 2.46 | 0.51 |
| 36:RQ:32:TYR:OH | 36:RQ:111:GLU:HB3 | 2.10 | 0.51 |
| 36:RQ:4:PRO:HG3 | 36:RQ:69:PHE:HE2 | 1.76 | 0.51 |
| 40:RU:97:ASP:OD1 | 40:RU:101:ARG:NH1 | 2.44 | 0.51 |
| 40:RU:36:ARG:HG2 | 40:RU:40:PHE:CE2 | 2.46 | 0.51 |
| 1:XA:1437:C:H2' | 1:XA:1438:G:H8 | 1.75 | 0.51 |
| 1:XA:116:A:H61 | 1:XA:313:A:H1' | 1.75 | 0.51 |
| 1:XA:437:U:H2' | 1:XA:438:G:O4' | 2.11 | 0.51 |
| 19:XS:3:ARG:HH21 | 19:XS:7:LYS:HD2 | 1.76 | 0.51 |
| 19:XS:31:ILE:HG23 | 19:XS:49:ILE:HA | 1.92 | 0.51 |
| 25:YA:2331:G:O2' | 46:Y0:43:THR:HG22 | 2.11 | 0.51 |
| 25:YA:1263:U:H2' | 25:YA:1264:G:C8 | 2.46 | 0.51 |
| 25:YA:172:C:H2' | 25:YA:173:G:H8 | 1.74 | 0.51 |
| 25:YA:1754:C:P | 39:YT:96:ARG:HH12 | 2.34 | 0.51 |
| 25:YA:1779:U:OP2 | 25:YA:1784:A:N6 | 2.32 | 0.51 |
| 25:YA:2071:A:H2' | 25:YA:2072:G:H8 | 1.75 | 0.51 |
| 28:YE:115:GLY:HA2 | 28:YE:157:ALA:HB1 | 1.93 | 0.51 |
| 32:YI:4:ILE:HG12 | 32:YI:18:VAL:HG22 | 1.91 | 0.51 |
| 37:YR:104:ARG:HG3 | 37:YR:107:ASP:HB3 | 1.92 | 0.51 |
| 3:QC:150:LYS:HB3 | 3:QC:201:TYR:HB2 | 1.93 | 0.51 |
| 3:QC:70:VAL:HG12 | 3:QC:72:LYS:H | 1.75 | 0.51 |
| 10:QJ:4:ILE:HG12 | 10:QJ:100:THR:HG22 | 1.92 | 0.51 |
| 13:QM:93:ARG:HD2 | 13:QM:94:ARG:NH1 | 2.26 | 0.51 |
| 22:QW:11:A:H2' | 22:QW:12:G:C8 | 2.46 | 0.51 |
| 25:RA:1329:U:H5'' | 25:RA:1330:C:C5 | 2.45 | 0.51 |
| 25:RA:1465:G:H4' | 25:RA:1528:A:H1' | 1.93 | 0.51 |
| 25:RA:1972:A:H2' | 25:RA:1973:G:H8 | 1.75 | 0.51 |
| 25:RA:2526:G:O2' | 55:R9:3:VAL:HB | 2.11 | 0.51 |
| 25:RA:811:U:H2' | 35:RP:21:ARG:O | 2.11 | 0.51 |
| 1:XA:1437:C:H2' | 1:XA:1438:G:C8 | 2.46 | 0.51 |
| 1:XA:152:A:H62 | 1:XA:169:C:H42 | 1.58 | 0.51 |
| 1:XA:78:G:H2' | 1:XA:79:G:C8 | 2.46 | 0.51 |
| 11:XK:33:THR:HG22 | 11:XK:39:PRO:HA | 1.93 | 0.51 |
| 25:YA:1570:A:H2' | 25:YA:1571:A:C8 | 2.46 | 0.51 |
| 25:YA:222:A:H3' | 25:YA:421:U:H5' | 1.92 | 0.51 |
| 25:YA:2247:A:H2' | 25:YA:2248:C:C6 | 2.46 | 0.51 |
| 25:YA:662:G:H2' | 25:YA:663:G:H8 | 1.75 | 0.51 |
| 25:YA:864:G:H2' | 25:YA:865:C:C6 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:968:G:H2' | 25:YA:969:U:C6 | 2.46 | 0.51 |
| 27:YD:182:LEU:H | 27:YD:272:ALA:HB3 | 1.75 | 0.51 |
| 31:YH:19:VAL:HA | 31:YH:24:VAL:HG12 | 1.92 | 0.51 |
| 1:QA:1004:A:OP1 | 1:QA:1025:U:N3 | 2.40 | 0.50 |
| 1:QA:368:U:OP1 | 32:YI:91:SER:OG | 2.23 | 0.50 |
| 1:QA:624:C:H2' | 1:QA:625:G:C8 | 2.45 | 0.50 |
| 1:QA:976:G:P | 14:QN:32:SER:H | 2.34 | 0.50 |
| 22:QV:44:A:H2' | 22:QV:45:A:H8 | 1.76 | 0.50 |
| 25:RA:1657:C:H5' | 28:RE:137:HIS:HE1 | 1.76 | 0.50 |
| 25:RA:1664:A:H61 | 25:RA:1996:C:H42 | 1.58 | 0.50 |
| 25:RA:1794:U:H2' | 25:RA:1795:C:H6 | 1.76 | 0.50 |
| 25:RA:1935:G:H1' | 25:RA:1964:G:N2 | 2.26 | 0.50 |
| 25:RA:2626:C:H2' | 25:RA:2627:G:C8 | 2.46 | 0.50 |
| 25:RA:2696:U:H2' | 25:RA:2697:G:H8 | 1.75 | 0.50 |
| 25:RA:2820:A:O2' | 25:RA:2821:A:OP1 | 2.28 | 0.50 |
| 25:RA:760:G:H2' | 25:RA:761:A:O4' | 2.10 | 0.50 |
| 25:RA:78:A:H2' | 25:RA:79:G:H8 | 1.75 | 0.50 |
| 25:RA:918:A:N3 | 26:RB:80:U:O2' | 2.35 | 0.50 |
| 26:RB:44:G:H1' | 26:RB:47:C:N4 | 2.26 | 0.50 |
| 30:RG:108:ASN:HA | 50:R4:37:SER:HB3 | 1.92 | 0.50 |
| 30:RG:124:SER:HB2 | 30:RG:131:TYR:CE1 | 2.45 | 0.50 |
| 1:XA:677:U:H3 | 1:XA:713:G:H22 | 1.57 | 0.50 |
| 1:XA:1073:U:O2 | 2:XB:104:ASN:ND2 | 2.43 | 0.50 |
| 11:XK:20:TYR:HE1 | 11:XK:83:ILE:HD12 | 1.75 | 0.50 |
| 25:YA:1230:C:H2' | 25:YA:1231:G:C8 | 2.42 | 0.50 |
| 25:YA:2616:C:H2' | 25:YA:2617:C:C6 | 2.44 | 0.50 |
| 27:YD:242:ARG:O | 27:YD:244:ARG:HG2 | 2.11 | 0.50 |
| 28:YE:106:GLY:HA3 | 28:YE:196:VAL:HG12 | 1.92 | 0.50 |
| 25:YA:338:G:OP1 | 44:YY:4:LYS:NZ | 2.43 | 0.50 |
| 1:QA:1077:G:N2 | 1:QA:1080:A:OP2 | 2.38 | 0.50 |
| 1:QA:1133:G:H2' | 1:QA:1134:G:H8 | 1.76 | 0.50 |
| 1:QA:452:A:H2' | 1:QA:453:A:H8 | 1.76 | 0.50 |
| 19:QS:45:VAL:HG13 | 19:QS:63:THR:HA | 1.93 | 0.50 |
| 25:RA:151:C:H2' | 25:RA:152:G:H8 | 1.75 | 0.50 |
| 25:RA:1570:A:H2' | 25:RA:1571:A:C8 | 2.45 | 0.50 |
| 25:RA:2471:C:H3' | 25:RA:2472:G:H8 | 1.76 | 0.50 |
| 25:RA:2853:C:H2' | 25:RA:2854:G:H8 | 1.76 | 0.50 |
| 25:RA:620:G:H4' | 25:RA:621:A:H5'' | 1.94 | 0.50 |
| 27:RD:35:LYS:HA | 27:RD:35:LYS:HE2 | 1.94 | 0.50 |
| 29:RF:116:ASP:OD2 | 35:RP:1:MET:N | 2.40 | 0.50 |
| 31:RH:106:THR:HG22 | 31:RH:112:PRO:HB3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:1652:A:OP1 | 37:RR:8:ARG:NH1 | 2.43 | 0.50 |
| 39:RT:111:ARG:C | 39:RT:113:LYS:H | 2.14 | 0.50 |
| 41:RV:60:GLU:HB2 | 41:RV:97:LYS:HE3 | 1.93 | 0.50 |
| 45:RZ:6:LYS:O | 45:RZ:62:PRO:HD3 | 2.10 | 0.50 |
| 1:XA:509:A:H4' | 1:XA:510:A:OP1 | 2.11 | 0.50 |
| 1:XA:911:U:H2' | 1:XA:912:C:C6 | 2.46 | 0.50 |
| 2:XB:19:HIS:CD2 | 2:XB:206:ASP:HB2 | 2.45 | 0.50 |
| 1:XA:1192:C:O2 | 5:XE:25:ARG:NH2 | 2.42 | 0.50 |
| 12:XL:45:PRO:HG3 | 12:XL:53:ARG:HD3 | 1.93 | 0.50 |
| 1:XA:1312:G:H5' | 19:XS:5:LEU:HD11 | 1.94 | 0.50 |
| 20:XT:29:LYS:O | 20:XT:33:ILE:HG12 | 2.11 | 0.50 |
| 25:YA:1568:G:OP2 | 27:YD:63:ARG:NH2 | 2.45 | 0.50 |
| 25:YA:2308:G:H1 | 25:YA:2311:A:H2 | 1.58 | 0.50 |
| 25:YA:2472:G:O2' | 25:YA:2478:A:N6 | 2.40 | 0.50 |
| 25:YA:2742:C:N3 | 55:Y9:33:LYS:NZ | 2.59 | 0.50 |
| 26:YB:29:A:H2' | 26:YB:30:C:C6 | 2.46 | 0.50 |
| 31:YH:69:ARG:NH1 | 31:YH:73:ALA:HB2 | 2.27 | 0.50 |
| 39:YT:91:ARG:HD2 | 39:YT:120:ARG:NH1 | 2.26 | 0.50 |
| 1:QA:456:C:H2' | 1:QA:457:C:H6 | 1.77 | 0.50 |
| 1:QA:736:C:H2' | 1:QA:737:A:C8 | 2.46 | 0.50 |
| 1:QA:1523:G:OP1 | 11:QK:123:LYS:NZ | 2.44 | 0.50 |
| 50:R4:11:PRO:HA | 50:R4:25:TYR:CD1 | 2.47 | 0.50 |
| 25:RA:1264:G:H3' | 25:RA:1265:A:H5'' | 1.93 | 0.50 |
| 25:RA:2243:U:H2' | 25:RA:2244:U:C6 | 2.46 | 0.50 |
| 25:RA:598:G:H4' | 35:RP:11:GLY:HA3 | 1.93 | 0.50 |
| 25:RA:95:G:O2' | 48:R2:48:HIS:ND1 | 2.35 | 0.50 |
| 28:RE:45:THR:O | 28:RE:83:ASP:N | 2.43 | 0.50 |
| 37:RR:17:ARG:HG2 | 37:RR:21:TYR:HE2 | 1.75 | 0.50 |
| 1:XA:539:A:H2' | 1:XA:540:G:C8 | 2.46 | 0.50 |
| 1:XA:652:U:O4 | 1:XA:752:G:O2' | 2.22 | 0.50 |
| 4:XD:173:TRP:CD1 | 4:XD:174:LEU:HG | 2.46 | 0.50 |
| 12:XL:53:ARG:HB3 | 12:XL:69:TYR:HE1 | 1.76 | 0.50 |
| 25:YA:191:A:H2' | 25:YA:192:C:H6 | 1.77 | 0.50 |
| 25:YA:2462:U:H2' | 25:YA:2463:C:C6 | 2.44 | 0.50 |
| 25:YA:304:G:H2' | 25:YA:305:U:C6 | 2.47 | 0.50 |
| 25:YA:720:C:H2' | 25:YA:721:C:H6 | 1.76 | 0.50 |
| 2:QB:19:HIS:HB2 | 2:QB:204:ASN:OD1 | 2.11 | 0.50 |
| 13:QM:23:TYR:N | 13:QM:67:GLU:OE2 | 2.38 | 0.50 |
| 16:QP:45:THR:HG22 | 16:QP:47:ASP:H | 1.77 | 0.50 |
| 25:RA:1794:U:H2' | 25:RA:1795:C:C6 | 2.47 | 0.50 |
| 25:RA:2689:U:H4' | 25:RA:2690:C:O5' | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:270(U):C:H2' | 25:RA:270(V):G:H8 | 1.76 | 0.50 |
| 25:RA:2747:G:N2 | 25:RA:2757:A:N6 | 2.28 | 0.50 |
| 26:RB:75:G:HO2' | 45:RZ:85:HIS:CD2 | 2.28 | 0.50 |
| 25:RA:1353:A:H4' | 27:RD:38:LYS:HE3 | 1.92 | 0.50 |
| 25:RA:2311:A:C8 | 30:RG:82:LEU:HD11 | 2.47 | 0.50 |
| 32:RI:133:HIS:HB3 | 32:RI:134:PRO:HD3 | 1.93 | 0.50 |
| 1:XA:115:G:H4' | 1:XA:116:A:O5' | 2.11 | 0.50 |
| 1:XA:1245:A:OP2 | 21:XU:9:ARG:NH2 | 2.44 | 0.50 |
| 3:XC:17:ASP:O | 3:XC:54:ARG:NH2 | 2.44 | 0.50 |
| 4:XD:18:LYS:HE2 | 4:XD:20:TYR:CZ | 2.47 | 0.50 |
| 17:XQ:51:TYR:CE2 | 17:XQ:73:VAL:HG11 | 2.46 | 0.50 |
| 25:YA:923:C:H4' | 46:Y0:29:GLN:HG3 | 1.93 | 0.50 |
| 25:YA:214:G:N3 | 25:YA:216:A:O2' | 2.37 | 0.50 |
| 25:YA:2744:G:C5 | 25:YA:2761:G:C6 | 3.00 | 0.50 |
| 25:YA:747:U:O2 | 25:YA:2014:A:H1' | 2.11 | 0.50 |
| 25:YA:969:U:H2' | 25:YA:970:C:C6 | 2.46 | 0.50 |
| 32:YI:100:ALA:O | 32:YI:104:GLN:CB | 2.59 | 0.50 |
| 36:YQ:55:VAL:HG13 | 45:YZ:178:GLU:HB3 | 1.93 | 0.50 |
| 1:QA:1305:G:HO2' | 1:QA:1306:A:H8 | 1.59 | 0.50 |
| 1:QA:877:C:OP1 | 8:QH:88:LYS:HE3 | 2.11 | 0.50 |
| 6:QF:44:GLY:HA2 | 6:QF:59:TYR:CE1 | 2.45 | 0.50 |
| 8:QH:34:GLU:OE1 | 8:QH:37:ARG:NH2 | 2.45 | 0.50 |
| 11:QK:54:ARG:HH22 | 22:QW:40:C:H4' | 1.76 | 0.50 |
| 16:QP:53:VAL:HG12 | 16:QP:79:VAL:HG22 | 1.93 | 0.50 |
| 25:RA:242:G:H3' | 54:R8:6:THR:HG23 | 1.93 | 0.50 |
| 25:RA:1952:A:C5 | 34:RO:22:ILE:HD12 | 2.46 | 0.50 |
| 25:RA:2623:G:OP1 | 25:RA:2826:A:O2' | 2.21 | 0.50 |
| 28:RE:115:GLY:HA2 | 28:RE:157:ALA:HB1 | 1.94 | 0.50 |
| 1:XA:1071:C:H2' | 1:XA:1072:G:H8 | 1.75 | 0.50 |
| 1:XA:191(E):G:H2' | 1:XA:191(F):U:C6 | 2.47 | 0.50 |
| 19:XS:10:PHE:HE2 | 19:XS:16:LEU:HD13 | 1.76 | 0.50 |
| 22:XW:10:G:H2' | 22:XW:11:A:C8 | 2.47 | 0.50 |
| 46:Y0:69:PHE:HE1 | 46:Y0:79:VAL:HG13 | 1.76 | 0.50 |
| 49:Y3:18:ASP:OD1 | 49:Y3:19:GLN:N | 2.44 | 0.50 |
| 25:YA:2247:A:H2' | 25:YA:2248:C:H6 | 1.77 | 0.50 |
| 25:YA:2701:C:H3' | 25:YA:2702:U:C5' | 2.38 | 0.50 |
| 25:YA:296:C:H2' | 25:YA:297:C:H6 | 1.76 | 0.50 |
| 25:YA:387:U:P | 47:Y1:20:ARG:HH12 | 2.34 | 0.50 |
| 25:YA:1490:A:O2' | 27:YD:99:ASP:OD1 | 2.29 | 0.50 |
| 25:YA:1649:G:O2' | 37:YR:107:ASP:OD1 | 2.17 | 0.50 |
| 1:QA:1372:U:H2' | 1:QA:1373:G:O4' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:QD:154:ASN:OD1 | 4:QD:155:LEU:N | 2.40 | 0.50 |
| 16:QP:69:THR:O | 16:QP:72:ARG:HG2 | 2.11 | 0.50 |
| 25:RA:1434:A:H61 | 25:RA:1558:A:H62 | 1.59 | 0.50 |
| 25:RA:1266:G:O2' | 25:RA:2012:G:O6 | 2.19 | 0.50 |
| 25:RA:995:C:O2 | 33:RN:3:THR:OG1 | 2.28 | 0.50 |
| 31:RH:9:ILE:HD13 | 31:RH:49:VAL:HG12 | 1.94 | 0.50 |
| 38:RS:20:ARG:HH22 | 46:R0:47:PRO:HB2 | 1.77 | 0.50 |
| 39:RT:91:ARG:HD2 | 39:RT:120:ARG:NH1 | 2.27 | 0.50 |
| 42:RW:111:HIS:CD2 | 42:RW:113:LYS:H | 2.29 | 0.50 |
| 1:XA:1336:C:H1' | 1:XA:1337:G:C2 | 2.47 | 0.50 |
| 1:XA:481:G:O2' | 1:XA:482:A:H8 | 1.95 | 0.50 |
| 5:XE:15:ARG:HD2 | 5:XE:26:PHE:CD2 | 2.47 | 0.50 |
| 16:XP:45:THR:HG22 | 16:XP:47:ASP:H | 1.76 | 0.50 |
| 25:YA:1400:G:H2' | 25:YA:1401:G:H8 | 1.76 | 0.50 |
| 25:YA:2741:A:N3 | 55:Y9:30:PRO:HD2 | 2.27 | 0.50 |
| 25:YA:2747:G:H1 | 25:YA:2755:C:P | 2.35 | 0.50 |
| 25:YA:938:G:H2' | 25:YA:939:G:H8 | 1.76 | 0.50 |
| 27:YD:35:LYS:HE2 | 27:YD:35:LYS:HA | 1.92 | 0.50 |
| 32:YI:14:ASP:C | 32:YI:16:GLY:H | 2.14 | 0.50 |
| 40:YU:108:GLU:HG3 | 41:YV:45:THR:OG1 | 2.11 | 0.50 |
| 43:YX:72:LYS:NZ | 43:YX:75:ASP:OD1 | 2.44 | 0.50 |
| 1:QA:370:C:H2' | 1:QA:371:G:C8 | 2.47 | 0.50 |
| 7:QG:22:LEU:HG | 7:QG:62:PHE:HE2 | 1.76 | 0.50 |
| 8:QH:82:HIS:HB3 | 8:QH:138:TRP:CE2 | 2.46 | 0.50 |
| 25:RA:2046:G:H5' | 51:R5:19:ARG:HG3 | 1.94 | 0.50 |
| 25:RA:194:G:H2' | 25:RA:195:A:O4' | 2.11 | 0.50 |
| 25:RA:2241:A:H2' | 25:RA:2242:G:H8 | 1.76 | 0.50 |
| 25:RA:2630:G:H2' | 25:RA:2631:G:H8 | 1.77 | 0.50 |
| 25:RA:2682:U:O2' | 39:RT:58:ASN:ND2 | 2.45 | 0.50 |
| 1:XA:1236:A:H2' | 1:XA:1237:C:C6 | 2.47 | 0.50 |
| 3:XC:130:VAL:O | 3:XC:134:ILE:HG12 | 2.11 | 0.50 |
| 25:YA:2329:G:H2' | 25:YA:2330:G:C8 | 2.46 | 0.50 |
| 8:QH:20:TYR:CE2 | 8:QH:75:ARG:HD2 | 2.47 | 0.50 |
| 13:QM:14:ARG:HH12 | 13:QM:42:ALA:HA | 1.76 | 0.50 |
| 14:QN:26:ARG:HD3 | 14:QN:43:CYS:HB3 | 1.94 | 0.50 |
| 25:RA:2852:G:H2' | 25:RA:2853:C:C6 | 2.46 | 0.50 |
| 27:RD:146:GLU:HB2 | 27:RD:189:CYS:HB3 | 1.92 | 0.50 |
| 29:RF:148:LEU:HD22 | 29:RF:154:VAL:HG21 | 1.93 | 0.50 |
| 38:RS:66:ALA:HA | 38:RS:69:VAL:HG12 | 1.93 | 0.50 |
| 42:RW:82:LEU:HD23 | 42:RW:84:ARG:NH2 | 2.26 | 0.50 |
| 44:RY:9:LYS:HE2 | 44:RY:28:LYS:O | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:RZ:4:ARG:HA | 45:RZ:59:LEU:H | 1.77 | 0.50 |
| 1:XA:1095:U:P | 1:XA:1108:G:H1 | 2.34 | 0.50 |
| 22:XV:35:C:O2' | 22:XV:36:A:OP1 | 2.29 | 0.50 |
| 25:YA:1022:G:N2 | 25:YA:1023:U:O4 | 2.44 | 0.50 |
| 25:YA:1408:C:H2' | 25:YA:1409:C:C6 | 2.47 | 0.50 |
| 25:YA:23:G:OP1 | 25:YA:504:U:N3 | 2.40 | 0.50 |
| 30:YG:15:VAL:HG21 | 30:YG:176:LEU:HD23 | 1.93 | 0.50 |
| 31:YH:130:ARG:NH1 | 31:YH:132:ARG:HE | 2.09 | 0.50 |
| 35:YP:91:PHE:CE2 | 35:YP:95:VAL:HG22 | 2.47 | 0.50 |
| 1:QA:414:A:OP2 | 1:QA:428:G:N2 | 2.43 | 0.50 |
| 8:QH:12:ARG:HD2 | 8:QH:26:VAL:HG12 | 1.93 | 0.50 |
| 10:QJ:48:THR:HA | 10:QJ:62:HIS:HB3 | 1.93 | 0.50 |
| 28:RE:101:ARG:NH1 | 28:RE:171:GLU:HB2 | 2.26 | 0.50 |
| 32:RI:69:LYS:HG3 | 32:RI:136:VAL:HG23 | 1.94 | 0.50 |
| 33:RN:47:ALA:HB2 | 33:RN:112:LEU:HD11 | 1.94 | 0.50 |
| 1:XA:1062:U:H2' | 1:XA:1063:C:C6 | 2.47 | 0.50 |
| 1:XA:1376:U:OP1 | 7:XG:98:SER:OG | 2.25 | 0.50 |
| 1:XA:920:U:H2' | 1:XA:921:U:C6 | 2.46 | 0.50 |
| 4:XD:30:LYS:HG2 | 4:XD:35:ARG:HH21 | 1.76 | 0.50 |
| 12:XL:32:PHE:HE1 | 12:XL:86:ARG:HG3 | 1.77 | 0.50 |
| 19:XS:10:PHE:CD1 | 19:XS:38:SER:HB2 | 2.47 | 0.50 |
| 22:XV:37:U:H2' | 22:XV:38:A:H8 | 1.77 | 0.50 |
| 25:YA:1167:U:H2' | 25:YA:1168:G:C8 | 2.47 | 0.50 |
| 25:YA:2630:G:H2' | 25:YA:2631:G:C8 | 2.47 | 0.50 |
| 25:YA:273:G:H2' | 25:YA:273(A):G:H8 | 1.77 | 0.50 |
| 25:YA:2747:G:H21 | 25:YA:2757:A:H62 | 1.58 | 0.50 |
| 25:YA:582:G:H2' | 25:YA:583:G:C8 | 2.47 | 0.50 |
| 25:YA:764:A:N3 | 27:YD:213:ARG:NH1 | 2.60 | 0.50 |
| 25:YA:823:G:H2' | 25:YA:824:A:C8 | 2.45 | 0.50 |
| 27:YD:36:PRO:HD3 | 27:YD:63:ARG:HG3 | 1.94 | 0.50 |
| 31:YH:150:ALA:O | 55:Y9:19:ARG:HD3 | 2.12 | 0.50 |
| 32:YI:133:HIS:HB3 | 32:YI:134:PRO:HD3 | 1.94 | 0.50 |
| 42:YW:45:TYR:CZ | 42:YW:49:LYS:HD2 | 2.47 | 0.50 |
| 1:QA:1071:C:H2' | 1:QA:1072:G:C8 | 2.45 | 0.49 |
| 1:QA:1169:A:H2' | 1:QA:1170:A:C8 | 2.47 | 0.49 |
| 1:QA:1222:G:OP1 | 19:QS:78:ARG:NH1 | 2.34 | 0.49 |
| 1:QA:1527:C:H2' | 1:QA:1528:U:C6 | 2.47 | 0.49 |
| 1:QA:272:C:H2' | 1:QA:273:A:C8 | 2.47 | 0.49 |
| 1:QA:688:G:H2' | 1:QA:689:C:C6 | 2.47 | 0.49 |
| 5:QE:91:LEU:HG | 5:QE:120:THR:HG22 | 1.94 | 0.49 |
| 1:QA:1346:A:N3 | 9:QI:107:ARG:NH2 | 2.59 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:R1:44:PRO:HG2 | 47:R1:46:LEU:CD1 | 2.42 | 0.49 |
| 25:RA:144:C:H2' | 25:RA:145:G:C8 | 2.46 | 0.49 |
| 25:RA:1791:A:H8 | 25:RA:1791:A:OP2 | 1.95 | 0.49 |
| 25:RA:1804:C:OP1 | 27:RD:259:THR:OG1 | 2.30 | 0.49 |
| 40:RU:83:LEU:HD12 | 40:RU:113:ALA:HB2 | 1.93 | 0.49 |
| 1:XA:923:A:O2' | 1:XA:1399:C:OP2 | 2.27 | 0.49 |
| 1:XA:482:A:H2' | 1:XA:483:C:O4' | 2.12 | 0.49 |
| 25:YA:1055:G:O2' | 25:YA:1085:A:N1 | 2.28 | 0.49 |
| 25:YA:1453:A:N6 | 25:YA:2702:U:H1' | 2.27 | 0.49 |
| 25:YA:1923:U:H2' | 25:YA:1924:C:C6 | 2.47 | 0.49 |
| 25:YA:676:A:C8 | 25:YA:2070:G:H1' | 2.47 | 0.49 |
| 25:YA:227:A:C2 | 25:YA:2407:G:H1' | 2.47 | 0.49 |
| 25:YA:2692:C:H2' | 25:YA:2693:A:H8 | 1.77 | 0.49 |
| 25:YA:2698:U:H2' | 25:YA:2699:C:C6 | 2.47 | 0.49 |
| 25:YA:2868:A:H2' | 25:YA:2869:G:C8 | 2.46 | 0.49 |
| 30:YG:106:LEU:HD12 | 30:YG:110:ALA:HB3 | 1.94 | 0.49 |
| 30:YG:107:LEU:HD23 | 30:YG:111:LEU:HD12 | 1.93 | 0.49 |
| 39:YT:123:GLN:O | 39:YT:126:ALA:N | 2.40 | 0.49 |
| 39:YT:26:ASP:HB3 | 39:YT:92:GLY:H | 1.76 | 0.49 |
| 43:YX:57:LEU:HD11 | 43:YX:78:LYS:HD2 | 1.94 | 0.49 |
| 1:QA:936:C:C2 | 1:QA:937:A:C8 | 3.01 | 0.49 |
| 3:QC:138:VAL:HG13 | 3:QC:149:ALA:HB3 | 1.94 | 0.49 |
| 19:QS:23:ASN:OD1 | 19:QS:24:ALA:N | 2.45 | 0.49 |
| 22:QW:71:G:H21 | 25:RA:1851:U:H4' | 1.76 | 0.49 |
| 54:R8:29:LYS:HB2 | 54:R8:33:ASN:ND2 | 2.27 | 0.49 |
| 25:RA:2478:A:H5'' | 55:R9:5:ALA:HB3 | 1.94 | 0.49 |
| 25:RA:1791:A:H5' | 27:RD:206:LEU:HD12 | 1.93 | 0.49 |
| 25:RA:2059:A:H5' | 25:RA:2060:A:OP2 | 2.13 | 0.49 |
| 25:RA:2403:C:C2 | 25:RA:2415:G:C2 | 2.99 | 0.49 |
| 25:RA:271(B):G:H1 | 25:RA:404:C:H42 | 1.60 | 0.49 |
| 26:RB:111:U:H2' | 26:RB:112:G:H8 | 1.77 | 0.49 |
| 25:RA:322:A:OP2 | 29:RF:169:ASN:HB2 | 2.12 | 0.49 |
| 32:RI:100:ALA:O | 32:RI:104:GLN:CB | 2.60 | 0.49 |
| 1:XA:244:U:H4' | 1:XA:245:C:O5' | 2.13 | 0.49 |
| 1:XA:993:G:O2' | 1:XA:994:A:N7 | 2.40 | 0.49 |
| 2:XB:212:GLN:HG3 | 2:XB:235:SER:HB2 | 1.93 | 0.49 |
| 13:XM:3:ARG:HD2 | 13:XM:9:ILE:HG12 | 1.94 | 0.49 |
| 25:YA:1076:C:H2' | 25:YA:1077:A:H5'' | 1.94 | 0.49 |
| 25:YA:2115:G:N2 | 25:YA:2165:G:N7 | 2.45 | 0.49 |
| 25:YA:2726:U:H5' | 34:YO:32:TYR:HE2 | 1.77 | 0.49 |
| 25:YA:587:C:H4' | 25:YA:588:U:O5' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:YD:36:PRO:HB2 | 27:YD:61:LEU:HB3 | 1.94 | 0.49 |
| 30:YG:81:LYS:O | 30:YG:82:LEU:HB2 | 2.12 | 0.49 |
| 43:YX:21:PHE:HA | 43:YX:26:TYR:HE1 | 1.76 | 0.49 |
| 1:QA:1402:C:H2' | 1:QA:1403:C:O4' | 2.12 | 0.49 |
| 5:QE:15:ARG:HG3 | 5:QE:28:PHE:HE1 | 1.77 | 0.49 |
| 1:QA:972:C:OP2 | 10:QJ:57:LYS:HG2 | 2.12 | 0.49 |
| 19:QS:10:PHE:CE2 | 19:QS:16:LEU:HB2 | 2.47 | 0.49 |
| 25:RA:1263:U:H2' | 25:RA:1264:G:C8 | 2.48 | 0.49 |
| 25:RA:1543:A:H1' | 25:RA:1545:A:O4' | 2.12 | 0.49 |
| 25:RA:242:G:H2' | 54:R8:5:LYS:HA | 1.95 | 0.49 |
| 25:RA:270(S):G:H21 | 47:R1:78:LYS:HE3 | 1.77 | 0.49 |
| 31:RH:115:VAL:HB | 31:RH:148:ILE:HD13 | 1.93 | 0.49 |
| 34:RO:104:ARG:HH11 | 34:RO:121:VAL:HG12 | 1.77 | 0.49 |
| 36:RQ:116:GLU:O | 36:RQ:120:ILE:HG12 | 2.12 | 0.49 |
| 36:RQ:135:ASP:OD2 | 45:RZ:81:ARG:NH2 | 2.40 | 0.49 |
| 39:RT:121:ILE:O | 39:RT:125:ARG:HG2 | 2.12 | 0.49 |
| 25:RA:1224:G:O6 | 41:RV:69:LYS:NZ | 2.45 | 0.49 |
| 1:XA:1308:U:H2' | 1:XA:1309:G:H8 | 1.76 | 0.49 |
| 1:XA:1357:A:H61 | 1:XA:1365:G:H1 | 1.60 | 0.49 |
| 1:XA:1392:G:H21 | 1:XA:1502:A:H8 | 1.58 | 0.49 |
| 1:XA:489:C:H2' | 1:XA:490:G:H8 | 1.76 | 0.49 |
| 6:XF:12:PRO:HG3 | 6:XF:57:GLN:HG3 | 1.94 | 0.49 |
| 9:XI:112:LYS:HA | 9:XI:119:ALA:HB2 | 1.94 | 0.49 |
| 22:XW:8:U:H2' | 22:XW:13:C:H41 | 1.77 | 0.49 |
| 47:Y1:86:SER:N | 47:Y1:87:PRO:HD2 | 2.27 | 0.49 |
| 25:YA:1184:G:OP1 | 49:Y3:30:ARG:HD2 | 2.12 | 0.49 |
| 25:YA:2361:A:O5' | 54:Y8:27:THR:OG1 | 2.29 | 0.49 |
| 25:YA:2742:C:H4' | 55:Y9:27:CYS:HB2 | 1.93 | 0.49 |
| 25:YA:1140:C:OP1 | 33:YN:23:LEU:HB3 | 2.12 | 0.49 |
| 25:YA:1204:A:O2' | 25:YA:1205:U:H5'' | 2.11 | 0.49 |
| 25:YA:2025:C:H2' | 25:YA:2026:C:C6 | 2.48 | 0.49 |
| 25:YA:820:A:H4' | 25:YA:836:G:N2 | 2.27 | 0.49 |
| 33:YN:70:LYS:HD3 | 33:YN:87:LEU:HD12 | 1.94 | 0.49 |
| 36:YQ:48:GLU:OE2 | 36:YQ:51:ARG:NH2 | 2.44 | 0.49 |
| 45:YZ:94:GLU:HB2 | 45:YZ:95:PRO:HD3 | 1.94 | 0.49 |
| 1:QA:129(A):G:N2 | 1:QA:188:U:O2' | 2.45 | 0.49 |
| 11:QK:82:VAL:HB | 11:QK:108:ILE:HG12 | 1.94 | 0.49 |
| 50:R4:45:GLY:C | 50:R4:47:GLN:H | 2.15 | 0.49 |
| 25:RA:1539:G:H2' | 25:RA:1540:G:H8 | 1.78 | 0.49 |
| 25:RA:2074:U:H2' | 25:RA:2075:U:H6 | 1.78 | 0.49 |
| 25:RA:2591:C:H2' | 25:RA:2592:G:H8 | 1.75 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2693:A:H2' | 25:RA:2694:G:H8 | 1.76 | 0.49 |
| 25:RA:30:G:H2' | 25:RA:31:C:C6 | 2.48 | 0.49 |
| 25:RA:607:U:OP1 | 29:RF:102:PRO:HA | 2.12 | 0.49 |
| 30:RG:120:LEU:HB2 | 30:RG:180:PHE:HD1 | 1.78 | 0.49 |
| 30:RG:67:LYS:HD2 | 30:RG:68:PRO:HD2 | 1.94 | 0.49 |
| 37:RR:74:LYS:C | 37:RR:76:VAL:H | 2.15 | 0.49 |
| 45:RZ:137:ILE:HG22 | 45:RZ:139:VAL:HG13 | 1.94 | 0.49 |
| 1:XA:337:C:H2' | 1:XA:338:A:C8 | 2.48 | 0.49 |
| 1:XA:559:A:H4' | 1:XA:560:U:H3' | 1.94 | 0.49 |
| 13:XM:91:ARG:HB2 | 13:XM:98:VAL:HG22 | 1.94 | 0.49 |
| 25:YA:2525:G:H1' | 55:Y9:28:GLU:HB2 | 1.94 | 0.49 |
| 25:YA:2574:G:H2' | 25:YA:2575:C:O4' | 2.12 | 0.49 |
| 25:YA:2743:C:H1' | 25:YA:2744:G:OP1 | 2.12 | 0.49 |
| 28:YE:50:GLY:HA2 | 28:YE:77:ILE:HA | 1.94 | 0.49 |
| 2:QB:74:LYS:NZ | 2:QB:205:ASP:O | 2.41 | 0.49 |
| 8:QH:17:THR:HB | 8:QH:78:GLN:OE1 | 2.12 | 0.49 |
| 20:QT:15:ARG:NH2 | 20:QT:18:GLN:OE1 | 2.46 | 0.49 |
| 1:QA:1453:G:C6 | 20:QT:55:ILE:HD11 | 2.47 | 0.49 |
| 25:RA:1667:G:O2' | 25:RA:1991:U:O4 | 2.30 | 0.49 |
| 25:RA:729:G:OP2 | 27:RD:13:ARG:HD3 | 2.13 | 0.49 |
| 25:RA:2635:C:O2' | 28:RE:80:GLU:OE2 | 2.30 | 0.49 |
| 30:RG:9:ARG:O | 30:RG:13:GLU:HG2 | 2.13 | 0.49 |
| 32:RI:78:THR:HG22 | 32:RI:141:LYS:HE3 | 1.93 | 0.49 |
| 25:RA:245:G:OP1 | 35:RP:69:GLY:HA3 | 2.13 | 0.49 |
| 49:Y3:11:SER:OG | 49:Y3:13:ILE:HG12 | 2.13 | 0.49 |
| 25:YA:1636:C:H2' | 25:YA:1637:A:H8 | 1.78 | 0.49 |
| 25:YA:1656:C:H2' | 25:YA:1657:C:H6 | 1.78 | 0.49 |
| 25:YA:1668:A:N3 | 25:YA:1670:C:N4 | 2.60 | 0.49 |
| 25:YA:2001:A:H2' | 25:YA:2002:G:C8 | 2.47 | 0.49 |
| 25:YA:2106:G:H2' | 25:YA:2107:C:C6 | 2.47 | 0.49 |
| 25:YA:2306:C:H3' | 25:YA:2307:G:H5'' | 1.93 | 0.49 |
| 25:YA:2743:C:O2' | 25:YA:2744:G:P | 2.70 | 0.49 |
| 25:YA:2747:G:H1' | 31:YH:67:LEU:HD12 | 1.94 | 0.49 |
| 25:YA:2756:U:O4 | 25:YA:2758:A:C5 | 2.65 | 0.49 |
| 25:YA:831:G:N2 | 35:YP:53:GLY:O | 2.45 | 0.49 |
| 38:YS:3:ARG:HE | 38:YS:4:LEU:HD13 | 1.77 | 0.49 |
| 1:QA:56:U:H2' | 1:QA:57:G:H8 | 1.78 | 0.49 |
| 1:QA:743:U:H2' | 1:QA:744:C:C6 | 2.47 | 0.49 |
| 1:QA:1104:G:H4' | 2:QB:111:ARG:HD2 | 1.93 | 0.49 |
| 2:QB:118:LEU:HB3 | 2:QB:142:LEU:HD12 | 1.93 | 0.49 |
| 25:RA:1019:U:HO2' | 25:RA:1021:A:H2 | 1.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1266:G:O5' | 42:RW:15:ARG:NH2 | 2.45 | 0.49 |
| 25:RA:270(J):G:H2' | 25:RA:270(K):C:O4' | 2.13 | 0.49 |
| 25:RA:2725:A:O2' | 25:RA:2726:U:H5'' | 2.12 | 0.49 |
| 25:RA:2303:G:O2' | 30:RG:132:ASN:HB2 | 2.13 | 0.49 |
| 31:RH:8:PRO:CG | 31:RH:69:ARG:HE | 2.15 | 0.49 |
| 34:RO:47:ILE:HG13 | 34:RO:48:PRO:HD2 | 1.95 | 0.49 |
| 36:RQ:4:PRO:HG3 | 36:RQ:69:PHE:CE2 | 2.48 | 0.49 |
| 1:XA:360:A:H2' | 1:XA:361:G:C8 | 2.46 | 0.49 |
| 1:XA:485:G:H1' | 1:XA:486:U:H5 | 1.77 | 0.49 |
| 1:XA:992:U:O2' | 1:XA:993:G:OP2 | 2.27 | 0.49 |
| 25:YA:1202:C:N4 | 25:YA:1203:G:C6 | 2.80 | 0.49 |
| 25:YA:1636:C:H2' | 25:YA:1637:A:C8 | 2.47 | 0.49 |
| 25:YA:2575:C:H5' | 28:YE:144:ARG:HG3 | 1.95 | 0.49 |
| 25:YA:29:U:H2' | 25:YA:30:G:H8 | 1.77 | 0.49 |
| 25:YA:836:G:H2' | 25:YA:837:C:H6 | 1.78 | 0.49 |
| 25:YA:92:G:H2' | 25:YA:93:C:C6 | 2.47 | 0.49 |
| 33:YN:47:ALA:O | 33:YN:119:ARG:NH1 | 2.40 | 0.49 |
| 1:QA:1309:G:C6 | 1:QA:1329:A:N1 | 2.81 | 0.49 |
| 1:QA:560:U:H4' | 1:QA:561:U:H5'' | 1.94 | 0.49 |
| 25:RA:1113:U:H2' | 25:RA:1114:G:H8 | 1.77 | 0.49 |
| 25:RA:1427:A:H4' | 25:RA:1428:C:O5' | 2.12 | 0.49 |
| 25:RA:1689:A:OP2 | 25:RA:1698:A:N6 | 2.41 | 0.49 |
| 25:RA:2341:G:H2' | 25:RA:2342:C:C6 | 2.47 | 0.49 |
| 25:RA:270(R):G:H2' | 25:RA:270(S):G:C8 | 2.48 | 0.49 |
| 25:RA:39:C:O2 | 29:RF:46:ARG:NH2 | 2.44 | 0.49 |
| 25:RA:546:C:H3' | 25:RA:547:A:H8 | 1.77 | 0.49 |
| 36:RQ:67:ARG:HD2 | 36:RQ:105:GLU:OE1 | 2.11 | 0.49 |
| 37:RR:88:ARG:NH2 | 37:RR:89:ASP:OD1 | 2.46 | 0.49 |
| 39:RT:39:ARG:HG2 | 39:RT:40:THR:H | 1.78 | 0.49 |
| 1:XA:1096:C:H2' | 1:XA:1097:C:H6 | 1.77 | 0.49 |
| 1:XA:375:U:O2' | 16:XP:6:LEU:O | 2.31 | 0.49 |
| 4:XD:108:LEU:HD21 | 4:XD:183:GLY:HA3 | 1.94 | 0.49 |
| 1:XA:599:C:O2' | 8:XH:129:VAL:O | 2.22 | 0.49 |
| 12:XL:24:VAL:HG13 | 12:XL:98:TYR:CE1 | 2.47 | 0.49 |
| 1:XA:254:G:O2' | 17:XQ:16:GLN:O | 2.28 | 0.49 |
| 24:XY:30:G:C2 | 24:XY:31:A:C8 | 3.01 | 0.49 |
| 25:YA:1062:G:N3 | 25:YA:1077:A:N6 | 2.61 | 0.49 |
| 25:YA:2037:G:H2' | 25:YA:2038:G:H8 | 1.76 | 0.49 |
| 25:YA:2290:G:H2' | 25:YA:2291:U:C6 | 2.47 | 0.49 |
| 25:YA:2512:C:H2' | 25:YA:2513:G:O4' | 2.12 | 0.49 |
| 25:YA:590:A:H2' | 25:YA:591:C:C6 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:YD:133:LEU:HB3 | 27:YD:173:VAL:HG21 | 1.94 | 0.49 |
| 29:YF:125:LEU:HA | 29:YF:194:MET:O | 2.12 | 0.49 |
| 31:YH:164:TYR:CD2 | 31:YH:167:GLU:HB2 | 2.47 | 0.49 |
| 32:YI:69:LYS:HG3 | 32:YI:136:VAL:HG23 | 1.95 | 0.49 |
| 32:YI:72:LEU:HD11 | 32:YI:101:LEU:HD11 | 1.95 | 0.49 |
| 33:YN:16:ILE:HG21 | 33:YN:26:LEU:HD11 | 1.95 | 0.49 |
| 36:YQ:39:PRO:HB3 | 36:YQ:99:PRO:HD3 | 1.95 | 0.49 |
| 40:YU:92:ARG:CD | 41:YV:11:GLN:HB2 | 2.40 | 0.49 |
| 1:QA:1414:U:H2' | 1:QA:1415:G:H8 | 1.78 | 0.49 |
| 1:QA:1399:C:C2 | 1:QA:1502:A:N6 | 2.81 | 0.49 |
| 1:QA:464:G:C6 | 1:QA:466:C:H5' | 2.48 | 0.49 |
| 1:QA:911:U:H2' | 1:QA:912:C:C6 | 2.48 | 0.49 |
| 25:RA:2210:G:H5' | 25:RA:2211:G:C6 | 2.48 | 0.49 |
| 25:RA:856:C:H2' | 25:RA:857:C:C6 | 2.48 | 0.49 |
| 37:RR:79:LEU:HD12 | 37:RR:83:ILE:HB | 1.95 | 0.49 |
| 42:RW:24:ILE:HD13 | 42:RW:36:LEU:HD11 | 1.94 | 0.49 |
| 1:XA:1522:U:H2' | 1:XA:1523:G:H8 | 1.77 | 0.49 |
| 1:XA:359:U:H2' | 1:XA:360:A:C8 | 2.48 | 0.49 |
| 1:XA:736:C:H2' | 1:XA:737:A:C8 | 2.46 | 0.49 |
| 5:XE:50:GLU:HB3 | 5:XE:53:LEU:HD13 | 1.95 | 0.49 |
| 22:XW:34:U:H3' | 22:XW:35:C:H5'' | 1.93 | 0.49 |
| 30:YG:179:PRO:HB3 | 50:Y4:43:TYR:CE1 | 2.48 | 0.49 |
| 25:YA:2064:C:H2' | 25:YA:2065:C:C6 | 2.47 | 0.49 |
| 25:YA:2379:G:O2' | 38:YS:17:ARG:NH2 | 2.35 | 0.49 |
| 25:YA:588:U:O4 | 25:YA:670:A:H1' | 2.13 | 0.49 |
| 29:YF:155:LEU:HB2 | 29:YF:189:THR:HG21 | 1.95 | 0.49 |
| 45:YZ:10:ARG:NH2 | 45:YZ:37:VAL:O | 2.46 | 0.49 |
| 1:QA:108:G:H5'' | 1:QA:109:A:H5'' | 1.94 | 0.49 |
| 1:QA:110:C:H2' | 1:QA:111:G:O4' | 2.12 | 0.49 |
| 1:QA:130:A:H5'' | 1:QA:190:G:H2' | 1.95 | 0.49 |
| 1:QA:385:C:H2' | 1:QA:386:C:C6 | 2.47 | 0.49 |
| 1:QA:32:A:H1' | 1:QA:48:C:H41 | 1.78 | 0.49 |
| 1:QA:579:G:H2' | 1:QA:580:U:C6 | 2.48 | 0.49 |
| 1:QA:64:G:H4' | 1:QA:65:U:O5' | 2.13 | 0.49 |
| 5:QE:50:GLU:HB3 | 5:QE:53:LEU:HD13 | 1.94 | 0.49 |
| 1:QA:1368:G:H4' | 14:QN:61:TRP:HZ2 | 1.78 | 0.49 |
| 25:RA:1140:C:OP2 | 33:RN:66:LYS:NZ | 2.31 | 0.49 |
| 25:RA:1164:G:H2' | 25:RA:1165:U:C6 | 2.47 | 0.49 |
| 25:RA:1351:C:O2' | 25:RA:1571:A:N3 | 2.37 | 0.49 |
| 25:RA:1991:U:H2' | 25:RA:1992:G:H5'' | 1.95 | 0.49 |
| 25:RA:2720:U:C2 | 25:RA:2721:A:C8 | 3.01 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:52:A:H2' | 25:RA:53:A:H8 | 1.78 | 0.49 |
| 25:RA:678:C:H2' | 25:RA:679:C:C6 | 2.48 | 0.49 |
| 25:RA:690:G:H2' | 25:RA:691:C:C6 | 2.48 | 0.49 |
| 26:RB:48:A:OP2 | 38:RS:30:ARG:NH2 | 2.46 | 0.49 |
| 34:RO:104:ARG:NH1 | 34:RO:121:VAL:O | 2.46 | 0.49 |
| 1:XA:1322:C:H5' | 13:XM:100:GLY:HA3 | 1.95 | 0.49 |
| 1:XA:20:U:H2' | 1:XA:21:G:O4' | 2.12 | 0.49 |
| 1:XA:555:C:H2' | 1:XA:556:C:H6 | 1.78 | 0.49 |
| 31:YH:149:ARG:C | 55:Y9:20:HIS:HB2 | 2.34 | 0.49 |
| 25:YA:2539:C:H1' | 55:Y9:29:ASN:ND2 | 2.27 | 0.49 |
| 25:YA:83:G:N1 | 25:YA:102:G:O2' | 2.31 | 0.49 |
| 25:YA:2004:G:C5 | 25:YA:2005:A:C8 | 3.01 | 0.49 |
| 25:YA:2329:G:H2' | 25:YA:2330:G:H8 | 1.78 | 0.49 |
| 25:YA:2455:G:H2' | 25:YA:2456:C:C6 | 2.48 | 0.49 |
| 25:YA:398:G:H2' | 25:YA:399:G:H8 | 1.78 | 0.49 |
| 25:YA:698:C:O2' | 25:YA:734:A:N6 | 2.45 | 0.49 |
| 27:YD:44:ASN:CB | 27:YD:49:ILE:HA | 2.43 | 0.49 |
| 1:QA:1145:C:H4' | 1:QA:1146:A:H8 | 1.78 | 0.49 |
| 22:QW:8:U:H2' | 22:QW:13:C:H41 | 1.78 | 0.49 |
| 25:RA:459:U:H4' | 53:R7:40:TRP:CZ3 | 2.48 | 0.49 |
| 54:R8:52:LYS:N | 54:R8:53:PRO:CD | 2.76 | 0.49 |
| 25:RA:278:A:H61 | 25:RA:362:U:H3 | 1.61 | 0.49 |
| 25:RA:627:A:H4' | 25:RA:628:G:H5' | 1.93 | 0.49 |
| 25:RA:859:G:N2 | 25:RA:917:A:OP2 | 2.46 | 0.49 |
| 28:RE:60:ASN:CG | 28:RE:62:PRO:HD2 | 2.33 | 0.49 |
| 30:RG:114:ILE:HB | 30:RG:117:PHE:HB2 | 1.95 | 0.49 |
| 1:XA:501:C:H2' | 1:XA:502:G:H8 | 1.78 | 0.49 |
| 1:XA:552:U:H2' | 1:XA:553:A:C8 | 2.48 | 0.49 |
| 1:XA:728:A:H2' | 1:XA:729:A:H8 | 1.76 | 0.49 |
| 5:XE:75:THR:HA | 5:XE:115:VAL:HG13 | 1.94 | 0.49 |
| 6:XF:80:ARG:HD2 | 6:XF:88:VAL:HB | 1.93 | 0.49 |
| 22:XW:5:G:H2' | 22:XW:6:G:C8 | 2.47 | 0.49 |
| 25:YA:1109:C:O2' | 25:YA:1110:G:OP1 | 2.28 | 0.49 |
| 25:YA:1800:C:H3' | 27:YD:147:LEU:HD22 | 1.95 | 0.49 |
| 25:YA:2541:A:HO2' | 25:YA:2764:A:H2 | 1.60 | 0.49 |
| 27:YD:77:ALA:HB3 | 27:YD:117:VAL:HG13 | 1.94 | 0.49 |
| 30:YG:170:ARG:NH2 | 30:YG:182:LYS:O | 2.46 | 0.49 |
| 1:QA:1443:G:C6 | 39:RT:118:ARG:HB2 | 2.48 | 0.48 |
| 1:QA:685:G:H21 | 1:QA:706:A:H61 | 1.61 | 0.48 |
| 2:QB:160:ASP:O | 2:QB:183:PRO:HD2 | 2.13 | 0.48 |
| 25:RA:2361:A:O5' | 54:R8:27:THR:OG1 | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2306:C:H3' | 25:RA:2307:G:H5'' | 1.95 | 0.48 |
| 25:RA:2698:U:H2' | 25:RA:2699:C:C6 | 2.48 | 0.48 |
| 25:RA:2771:C:H2' | 25:RA:2772:C:C6 | 2.48 | 0.48 |
| 25:RA:679:C:H2' | 25:RA:680:G:H8 | 1.78 | 0.48 |
| 28:RE:36:ARG:HG3 | 28:RE:47:VAL:HG12 | 1.95 | 0.48 |
| 34:RO:25:LEU:HB2 | 34:RO:38:VAL:HG13 | 1.95 | 0.48 |
| 38:RS:26:LEU:HD22 | 38:RS:87:PHE:HD1 | 1.78 | 0.48 |
| 41:RV:24:LYS:HD3 | 41:RV:90:PRO:HB2 | 1.93 | 0.48 |
| 1:XA:265:G:H2' | 1:XA:266:G:H5'' | 1.95 | 0.48 |
| 1:XA:552:U:O2 | 12:XL:31:PRO:HB3 | 2.12 | 0.48 |
| 13:XM:87:TYR:O | 13:XM:91:ARG:HG2 | 2.13 | 0.48 |
| 1:XA:663:A:H5'' | 18:XR:61:LYS:HE3 | 1.94 | 0.48 |
| 55:Y9:25:VAL:O | 55:Y9:33:LYS:HA | 2.13 | 0.48 |
| 25:YA:1638:C:O2 | 25:YA:2698:U:O2' | 2.29 | 0.48 |
| 25:YA:1853:A:N3 | 25:YA:2233:U:O2' | 2.40 | 0.48 |
| 25:YA:413:C:H2' | 25:YA:414:C:H6 | 1.76 | 0.48 |
| 25:YA:690:G:H4' | 27:YD:218:ARG:HH22 | 1.77 | 0.48 |
| 31:YH:120:GLY:HA3 | 31:YH:140:LYS:NZ | 2.28 | 0.48 |
| 39:YT:26:ASP:HB2 | 39:YT:90:GLN:O | 2.13 | 0.48 |
| 45:YZ:27:VAL:HG12 | 45:YZ:85:HIS:HE1 | 1.78 | 0.48 |
| 1:QA:1080:A:H5'' | 5:QE:16:THR:HG21 | 1.95 | 0.48 |
| 1:QA:320:C:H2' | 1:QA:321:A:C8 | 2.48 | 0.48 |
| 22:QV:24:C:H2' | 22:QV:25:U:C6 | 2.48 | 0.48 |
| 25:RA:517:C:OP1 | 51:R5:16:ARG:NH2 | 2.46 | 0.48 |
| 25:RA:1389:G:H2' | 25:RA:1390:U:C6 | 2.48 | 0.48 |
| 1:QA:1475:G:H4' | 25:RA:1689:A:H4' | 1.94 | 0.48 |
| 25:RA:1783:A:HO2' | 25:RA:2607:G:HO2' | 1.60 | 0.48 |
| 25:RA:263:C:H2' | 25:RA:264:C:O4' | 2.13 | 0.48 |
| 1:XA:1479:C:H2' | 1:XA:1480:G:C8 | 2.44 | 0.48 |
| 2:XB:25:ASN:ND2 | 2:XB:193:ASP:HB3 | 2.28 | 0.48 |
| 9:XI:125:TYR:CE2 | 9:XI:127:LYS:HB2 | 2.48 | 0.48 |
| 15:XO:67:LEU:HB3 | 15:XO:78:TYR:HE1 | 1.78 | 0.48 |
| 47:Y1:5:CYS:HB3 | 47:Y1:10:LYS:H | 1.77 | 0.48 |
| 50:Y4:45:GLY:C | 50:Y4:47:GLN:H | 2.16 | 0.48 |
| 25:YA:1689:A:H62 | 25:YA:1698:A:H2 | 1.61 | 0.48 |
| 25:YA:2133:G:O2' | 25:YA:2158:A:N1 | 2.41 | 0.48 |
| 25:YA:36:G:N3 | 25:YA:450:G:O2' | 2.44 | 0.48 |
| 25:YA:607:U:C5 | 25:YA:620:G:C5 | 3.01 | 0.48 |
| 25:YA:672:C:OP2 | 35:YP:42:SER:OG | 2.30 | 0.48 |
| 25:YA:755:C:H2' | 25:YA:756:C:H6 | 1.77 | 0.48 |
| 35:YP:33:ARG:HD3 | 35:YP:40:SER:HA | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1273:G:H3' | 1:QA:1274:G:H8 | 1.78 | 0.48 |
| 1:QA:1307:U:H2' | 1:QA:1308:U:C6 | 2.49 | 0.48 |
| 1:QA:191(E):G:H2' | 1:QA:191(F):U:C6 | 2.48 | 0.48 |
| 3:QC:17:ASP:O | 3:QC:54:ARG:NH2 | 2.45 | 0.48 |
| 22:QW:5:G:H2' | 22:QW:6:G:C8 | 2.49 | 0.48 |
| 25:RA:1078:U:HO2' | 25:RA:1079:C:P | 2.37 | 0.48 |
| 25:RA:2692:C:H2' | 25:RA:2693:A:H8 | 1.79 | 0.48 |
| 35:RP:37:GLY:O | 35:RP:41:ARG:HG2 | 2.14 | 0.48 |
| 35:RP:64:LYS:C | 35:RP:66:GLY:H | 2.17 | 0.48 |
| 25:RA:2406:U:N3 | 35:RP:72:PRO:HB2 | 2.28 | 0.48 |
| 25:RA:2250:G:C5 | 36:RQ:82:ARG:HG3 | 2.48 | 0.48 |
| 1:XA:1086:U:H3 | 1:XA:1099:G:N2 | 2.07 | 0.48 |
| 1:XA:1126:U:H1' | 1:XA:1280:A:C5 | 2.49 | 0.48 |
| 1:XA:1250:A:H2 | 1:XA:1370:G:H1' | 1.77 | 0.48 |
| 25:YA:17:G:H4' | 40:YU:25:TRP:NE1 | 2.25 | 0.48 |
| 25:YA:1858:G:O2' | 25:YA:1884:A:N6 | 2.46 | 0.48 |
| 25:YA:2693:A:H2' | 25:YA:2694:G:H8 | 1.78 | 0.48 |
| 25:YA:2741:A:O3' | 55:Y9:31:LYS:CB | 2.58 | 0.48 |
| 25:YA:795:C:H2' | 25:YA:796:C:C6 | 2.48 | 0.48 |
| 28:YE:74:PRO:HG2 | 28:YE:77:ILE:HG22 | 1.94 | 0.48 |
| 35:YP:57:THR:C | 35:YP:59:LEU:H | 2.17 | 0.48 |
| 25:YA:1243:G:H4' | 35:YP:7:ARG:HH21 | 1.78 | 0.48 |
| 45:YZ:150:LEU:HB2 | 45:YZ:154:ASP:OD2 | 2.14 | 0.48 |
| 1:QA:1137:C:O2' | 1:QA:1138:G:N3 | 2.46 | 0.48 |
| 1:QA:1152:A:H5'' | 10:QJ:13:HIS:CD2 | 2.48 | 0.48 |
| 1:QA:674:G:OP1 | 6:QF:87:ARG:NH2 | 2.45 | 0.48 |
| 6:QF:80:ARG:HD2 | 6:QF:88:VAL:HB | 1.95 | 0.48 |
| 25:RA:1496:A:H8 | 25:RA:1577:C:HO2' | 1.62 | 0.48 |
| 25:RA:2138:C:H42 | 25:RA:2153:G:H1 | 1.60 | 0.48 |
| 25:RA:2476:A:H2' | 25:RA:2477:C:H6 | 1.78 | 0.48 |
| 25:RA:2776:A:H4' | 25:RA:2777:G:O5' | 2.12 | 0.48 |
| 25:RA:634:C:H2' | 25:RA:635:C:C6 | 2.48 | 0.48 |
| 25:RA:909:A:H2' | 25:RA:912:C:H5 | 1.78 | 0.48 |
| 27:RD:61:LEU:O | 27:RD:63:ARG:NH1 | 2.39 | 0.48 |
| 1:XA:737:A:H2' | 1:XA:738:C:C6 | 2.48 | 0.48 |
| 2:XB:7:VAL:HG21 | 2:XB:217:ARG:HH11 | 1.79 | 0.48 |
| 1:XA:1350:A:O2' | 7:XG:33:ASP:OD1 | 2.29 | 0.48 |
| 9:XI:81:ILE:HG22 | 9:XI:85:LEU:HD23 | 1.96 | 0.48 |
| 48:Y2:17:SER:OG | 48:Y2:20:GLU:HG2 | 2.13 | 0.48 |
| 25:YA:1426:G:OP2 | 25:YA:1427:A:O2' | 2.25 | 0.48 |
| 25:YA:2152:G:H2' | 25:YA:2153:G:H8 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2363:C:O3' | 46:Y0:55:ARG:NH2 | 2.46 | 0.48 |
| 25:YA:2805:G:H2' | 25:YA:2807:G:C8 | 2.48 | 0.48 |
| 26:YB:15:A:H1' | 26:YB:109:G:C8 | 2.49 | 0.48 |
| 26:YB:33:G:H5' | 30:YG:2:PRO:CG | 2.41 | 0.48 |
| 26:YB:52:A:O2' | 26:YB:53:A:C8 | 2.66 | 0.48 |
| 28:YE:38:THR:OG1 | 28:YE:40:GLU:OE1 | 2.29 | 0.48 |
| 33:YN:34:LEU:O | 33:YN:49:GLY:HA3 | 2.14 | 0.48 |
| 43:YX:28:PHE:CE1 | 43:YX:92:LEU:HD11 | 2.49 | 0.48 |
| 45:YZ:137:ILE:HG22 | 45:YZ:139:VAL:HG13 | 1.96 | 0.48 |
| 1:QA:1129:C:H4' | 1:QA:1130:A:H8 | 1.79 | 0.48 |
| 1:QA:1200:C:O2' | 1:QA:1201:A:OP2 | 2.28 | 0.48 |
| 1:QA:399:G:H2' | 1:QA:400:C:H6 | 1.77 | 0.48 |
| 1:QA:922:G:H2' | 1:QA:923:A:C8 | 2.48 | 0.48 |
| 2:QB:77:ALA:HB2 | 2:QB:211:ILE:HD13 | 1.96 | 0.48 |
| 13:QM:40:ASN:HB3 | 13:QM:43:THR:HG23 | 1.95 | 0.48 |
| 25:RA:2419:U:H2' | 25:RA:2420:C:C6 | 2.48 | 0.48 |
| 25:RA:2465:C:H2' | 25:RA:2466:C:H5' | 1.96 | 0.48 |
| 26:RB:43:C:H4' | 30:RG:98:ARG:HH22 | 1.78 | 0.48 |
| 25:RA:1568:G:P | 27:RD:63:ARG:HH22 | 2.36 | 0.48 |
| 29:RF:117:ARG:HH21 | 29:RF:187:VAL:HA | 1.79 | 0.48 |
| 40:RU:44:ASN:HD21 | 41:RV:75:PHE:HB3 | 1.77 | 0.48 |
| 43:RX:28:PHE:CE1 | 43:RX:92:LEU:HD11 | 2.48 | 0.48 |
| 1:XA:1024:G:OP1 | 1:XA:1024:G:H4' | 2.13 | 0.48 |
| 1:XA:1189:C:P | 10:XJ:51:ARG:HH22 | 2.36 | 0.48 |
| 1:XA:1287:A:H2' | 1:XA:1288:A:H8 | 1.76 | 0.48 |
| 1:XA:1343:G:H1' | 9:XI:121:ARG:NH1 | 2.28 | 0.48 |
| 1:XA:1343:G:H2' | 1:XA:1344:C:C6 | 2.48 | 0.48 |
| 1:XA:137:C:O2' | 16:XP:61:SER:O | 2.31 | 0.48 |
| 1:XA:1521:G:H2' | 1:XA:1522:U:C6 | 2.49 | 0.48 |
| 2:XB:167:PRO:HG2 | 2:XB:192:SER:HB3 | 1.95 | 0.48 |
| 18:XR:31:LEU:H | 18:XR:31:LEU:HD23 | 1.78 | 0.48 |
| 18:XR:74:ARG:HG2 | 18:XR:81:PHE:CD1 | 2.49 | 0.48 |
| 19:XS:65:ASN:O | 50:Y4:58:ARG:HD2 | 2.13 | 0.48 |
| 22:XW:36:A:H2' | 22:XW:37:U:C6 | 2.49 | 0.48 |
| 31:YH:149:ARG:H | 55:Y9:20:HIS:CD2 | 2.31 | 0.48 |
| 25:YA:2153:G:H2' | 25:YA:2154:G:C8 | 2.48 | 0.48 |
| 25:YA:963:U:H2' | 25:YA:964:C:C6 | 2.49 | 0.48 |
| 28:YE:13:ARG:HA | 28:YE:22:PRO:HA | 1.96 | 0.48 |
| 28:YE:74:PRO:HG2 | 28:YE:77:ILE:CG2 | 2.44 | 0.48 |
| 30:YG:55:LYS:NZ | 30:YG:59:GLU:OE2 | 2.45 | 0.48 |
| 31:YH:142:GLY:O | 31:YH:146:ALA:CB | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:YT:120:ARG:O | 39:YT:123:GLN:HB2 | 2.14 | 0.48 |
| 1:QA:1258:G:H2' | 1:QA:1259:C:C6 | 2.48 | 0.48 |
| 1:QA:359:U:H2' | 1:QA:360:A:H8 | 1.78 | 0.48 |
| 1:QA:426:G:OP1 | 4:QD:38:TYR:OH | 2.31 | 0.48 |
| 1:QA:464:G:O6 | 1:QA:466:C:H5' | 2.14 | 0.48 |
| 4:QD:31:CYS:C | 4:QD:33:MET:H | 2.17 | 0.48 |
| 25:RA:2747:G:C2 | 25:RA:2757:A:N6 | 2.80 | 0.48 |
| 25:RA:2839:G:H1' | 37:RR:93:GLY:H | 1.78 | 0.48 |
| 25:RA:49:A:N7 | 25:RA:120:U:H5 | 2.12 | 0.48 |
| 25:RA:638:G:H2' | 25:RA:639:U:H6 | 1.78 | 0.48 |
| 25:RA:67:U:H2' | 25:RA:68:G:C8 | 2.49 | 0.48 |
| 25:RA:468:G:H4' | 29:RF:62:ARG:HH12 | 1.77 | 0.48 |
| 43:RX:18:TYR:HA | 43:RX:21:PHE:CD2 | 2.49 | 0.48 |
| 1:XA:322:C:H2' | 1:XA:323:U:C6 | 2.49 | 0.48 |
| 1:XA:539:A:H2' | 1:XA:540:G:H8 | 1.78 | 0.48 |
| 2:XB:82:ARG:NH1 | 2:XB:92:TYR:OH | 2.47 | 0.48 |
| 4:XD:131:ARG:HD3 | 4:XD:132:ARG:O | 2.14 | 0.48 |
| 1:XA:975:A:N1 | 10:XJ:48:THR:HB | 2.29 | 0.48 |
| 47:Y1:83:GLU:HG2 | 47:Y1:85:LEU:H | 1.78 | 0.48 |
| 49:Y3:11:SER:HB2 | 49:Y3:31:LEU:HD11 | 1.95 | 0.48 |
| 25:YA:1405:U:H2' | 25:YA:1406:U:H6 | 1.79 | 0.48 |
| 25:YA:2789:C:H1' | 25:YA:2892:A:C2 | 2.49 | 0.48 |
| 25:YA:374:A:H1' | 25:YA:401:A:N6 | 2.28 | 0.48 |
| 25:YA:857:C:OP1 | 46:Y0:69:PHE:HD2 | 1.96 | 0.48 |
| 30:YG:7:LEU:HD12 | 30:YG:10:LYS:HD2 | 1.96 | 0.48 |
| 36:YQ:32:TYR:OH | 36:YQ:111:GLU:HB3 | 2.13 | 0.48 |
| 39:YT:3:ARG:HG3 | 39:YT:7:ILE:HG12 | 1.95 | 0.48 |
| 39:YT:66:VAL:HA | 39:YT:71:GLY:HA2 | 1.95 | 0.48 |
| 1:QA:1144:G:H21 | 1:QA:1146:A:H62 | 1.62 | 0.48 |
| 1:QA:1292:U:H2' | 1:QA:1293:G:C8 | 2.48 | 0.48 |
| 1:QA:920:U:H2' | 1:QA:921:U:C6 | 2.48 | 0.48 |
| 4:QD:85:LYS:HD2 | 4:QD:92:VAL:HG11 | 1.95 | 0.48 |
| 13:QM:83:ASP:H | 13:QM:93:ARG:NH2 | 2.12 | 0.48 |
| 22:QW:36:A:H2' | 22:QW:37:U:C6 | 2.49 | 0.48 |
| 25:RA:1152:C:H4' | 40:RU:77:SER:HA | 1.96 | 0.48 |
| 25:RA:2037:G:H2' | 25:RA:2038:G:C8 | 2.49 | 0.48 |
| 25:RA:500:G:N1 | 25:RA:503:A:OP2 | 2.42 | 0.48 |
| 26:RB:32:C:C4 | 26:RB:51:G:N2 | 2.82 | 0.48 |
| 27:RD:43:ARG:HD2 | 27:RD:49:ILE:HD12 | 1.95 | 0.48 |
| 29:RF:107:LYS:HB3 | 29:RF:206:ILE:HD12 | 1.96 | 0.48 |
| 1:XA:545:C:O2' | 1:XA:549:C:OP1 | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:707:C:H2' | 1:XA:708:C:C6 | 2.49 | 0.48 |
| 4:XD:31:CYS:C | 4:XD:33:MET:H | 2.17 | 0.48 |
| 22:XW:10:G:H2' | 22:XW:11:A:H8 | 1.78 | 0.48 |
| 25:YA:1186:G:H8 | 25:YA:1186:G:O5' | 1.96 | 0.48 |
| 25:YA:220:G:O2' | 25:YA:233:A:N3 | 2.43 | 0.48 |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:H6 | 1.79 | 0.48 |
| 25:YA:2809:A:H2' | 25:YA:2810:A:C8 | 2.49 | 0.48 |
| 25:YA:2836:U:H2' | 25:YA:2837:G:H8 | 1.78 | 0.48 |
| 1:QA:1488:G:H2' | 1:QA:1489:G:C8 | 2.49 | 0.48 |
| 1:QA:433:C:H2' | 1:QA:434:U:H6 | 1.77 | 0.48 |
| 5:QE:102:ALA:HB1 | 5:QE:106:PRO:HG2 | 1.96 | 0.48 |
| 1:QA:778:G:O2' | 11:QK:120:ARG:O | 2.29 | 0.48 |
| 13:QM:87:TYR:HB2 | 19:QS:73:GLU:HA | 1.94 | 0.48 |
| 25:RA:1709:U:H2' | 25:RA:1710:C:C6 | 2.49 | 0.48 |
| 25:RA:2064:C:H2' | 25:RA:2065:C:H6 | 1.79 | 0.48 |
| 25:RA:974(A):C:H4' | 25:RA:975:G:C5' | 2.43 | 0.48 |
| 26:RB:109:G:H2' | 26:RB:110:G:H8 | 1.78 | 0.48 |
| 32:RI:14:ASP:C | 32:RI:16:GLY:H | 2.17 | 0.48 |
| 40:RU:92:ARG:CD | 41:RV:11:GLN:HB2 | 2.39 | 0.48 |
| 41:RV:61:VAL:HG12 | 41:RV:63:GLY:H | 1.77 | 0.48 |
| 1:XA:1055:A:N6 | 1:XA:1206:G:N7 | 2.62 | 0.48 |
| 1:XA:1314:C:H2' | 1:XA:1315:U:H6 | 1.79 | 0.48 |
| 1:XA:324:G:N2 | 1:XA:327:A:OP2 | 2.46 | 0.48 |
| 1:XA:69:G:HO2' | 1:XA:152:A:H2 | 1.60 | 0.48 |
| 13:XM:64:TRP:HD1 | 13:XM:65:LYS:O | 1.97 | 0.48 |
| 54:Y8:52:LYS:N | 54:Y8:53:PRO:CD | 2.77 | 0.48 |
| 25:YA:2744:G:O6 | 55:Y9:1:MET:SD | 2.71 | 0.48 |
| 25:YA:1332:G:N2 | 25:YA:1610:A:N7 | 2.59 | 0.48 |
| 25:YA:2764:A:N7 | 25:YA:2766:G:C5 | 2.82 | 0.48 |
| 25:YA:2795:G:H3' | 25:YA:2797:U:C5' | 2.43 | 0.48 |
| 28:YE:170:LEU:HD21 | 28:YE:187:ALA:HB3 | 1.96 | 0.48 |
| 30:YG:137:GLU:HB2 | 30:YG:152:LEU:HD22 | 1.96 | 0.48 |
| 31:YH:149:ARG:HE | 55:Y9:20:HIS:N | 2.06 | 0.48 |
| 37:YR:45:ARG:HA | 37:YR:95:THR:HG21 | 1.96 | 0.48 |
| 40:YU:74:LEU:HD12 | 40:YU:110:VAL:HG13 | 1.95 | 0.48 |
| 1:QA:1329:A:N7 | 21:QU:7:ARG:NH2 | 2.49 | 0.48 |
| 1:QA:1488:G:H2' | 1:QA:1489:G:H8 | 1.79 | 0.48 |
| 1:QA:514:C:H2' | 1:QA:515:G:H8 | 1.76 | 0.48 |
| 1:QA:981:U:H2' | 1:QA:982:U:C5 | 2.48 | 0.48 |
| 17:QQ:83:ASP:OD1 | 17:QQ:84:LEU:N | 2.45 | 0.48 |
| 25:RA:1065:U:O2 | 25:RA:1074:G:N1 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1336:A:H2' | 25:RA:1337:G:H8 | 1.79 | 0.48 |
| 25:RA:1869:G:H5' | 25:RA:1870:C:OP2 | 2.14 | 0.48 |
| 25:RA:922:U:H2' | 25:RA:923:C:C6 | 2.49 | 0.48 |
| 45:RZ:182:LYS:O | 45:RZ:182:LYS:HD3 | 2.14 | 0.48 |
| 1:XA:1036:G:H5' | 1:XA:1037:C:OP2 | 2.14 | 0.48 |
| 5:XE:15:ARG:HG3 | 5:XE:28:PHE:HE1 | 1.78 | 0.48 |
| 13:XM:14:ARG:HG2 | 13:XM:44:ARG:NH1 | 2.28 | 0.48 |
| 20:XT:89:ARG:HH21 | 20:XT:104:LEU:HD21 | 1.77 | 0.48 |
| 22:XW:1:C:H42 | 22:XW:73:A:H61 | 1.62 | 0.48 |
| 55:Y9:24:TYR:OH | 55:Y9:35:ARG:NE | 2.44 | 0.48 |
| 25:YA:1804:C:OP1 | 27:YD:259:THR:OG1 | 2.32 | 0.48 |
| 25:YA:2437:U:H2' | 25:YA:2438:U:C6 | 2.48 | 0.48 |
| 25:YA:2462:U:H2' | 25:YA:2463:C:H6 | 1.78 | 0.48 |
| 25:YA:401:A:H2' | 25:YA:402:A:C8 | 2.49 | 0.48 |
| 25:YA:755:C:H2' | 25:YA:756:C:C6 | 2.49 | 0.48 |
| 25:YA:783:A:H2' | 25:YA:784:A:H4' | 1.96 | 0.48 |
| 25:YA:1818:U:H2' | 27:YD:157:ARG:HG2 | 1.96 | 0.48 |
| 28:YE:35:GLN:HE21 | 28:YE:37:ARG:CZ | 2.26 | 0.48 |
| 29:YF:110:LEU:HD11 | 29:YF:181:LEU:HG | 1.96 | 0.48 |
| 31:YH:91:GLY:HA3 | 31:YH:94:TYR:CD2 | 2.49 | 0.48 |
| 43:YX:18:TYR:HA | 43:YX:21:PHE:CD2 | 2.49 | 0.48 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C8 | 2.49 | 0.48 |
| 1:QA:687:A:H2 | 1:QA:704:A:C6 | 2.32 | 0.48 |
| 1:QA:664:G:N2 | 1:QA:741:G:H1 | 2.08 | 0.48 |
| 9:QI:69:GLY:O | 9:QI:73:GLN:HG3 | 2.13 | 0.48 |
| 1:QA:973:G:C4 | 10:QJ:55:LYS:HE3 | 2.49 | 0.48 |
| 25:RA:1031:G:C2 | 55:R9:20:HIS:ND1 | 2.82 | 0.48 |
| 25:RA:1138:G:H21 | 33:RN:106:MET:HE3 | 1.79 | 0.48 |
| 25:RA:1201:C:H2' | 25:RA:1202:C:H6 | 1.78 | 0.48 |
| 25:RA:2233:U:H2' | 25:RA:2234:G:C8 | 2.49 | 0.48 |
| 25:RA:710:G:H2' | 25:RA:711:G:H8 | 1.78 | 0.48 |
| 25:RA:970:C:H2' | 25:RA:971:C:C6 | 2.49 | 0.48 |
| 25:RA:690:G:H21 | 27:RD:43:ARG:NH2 | 2.12 | 0.48 |
| 30:RG:60:LEU:HD21 | 30:RG:92:VAL:HG11 | 1.96 | 0.48 |
| 1:XA:1148:U:H2' | 1:XA:1149:C:O4' | 2.13 | 0.48 |
| 1:XA:114:U:H2' | 1:XA:115:G:C8 | 2.49 | 0.48 |
| 1:XA:138:G:H2' | 1:XA:139:G:C8 | 2.49 | 0.48 |
| 1:XA:21:G:H2' | 1:XA:22:G:H8 | 1.78 | 0.48 |
| 1:XA:411:A:N6 | 1:XA:413:G:H21 | 2.12 | 0.48 |
| 10:XJ:24:VAL:HG21 | 10:XJ:37:PRO:HG3 | 1.96 | 0.48 |
| 12:XL:45:PRO:HB3 | 12:XL:92:ASP:HB3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:XP:69:THR:O | 16:XP:72:ARG:HG2 | 2.13 | 0.48 |
| 47:Y1:52:ARG:HH11 | 47:Y1:57:GLU:HB2 | 1.79 | 0.48 |
| 25:YA:1165:U:H2' | 25:YA:1166:C:H6 | 1.79 | 0.48 |
| 25:YA:1301:A:C8 | 25:YA:1303:G:C8 | 3.01 | 0.48 |
| 25:YA:1688:U:H5' | 25:YA:1689:A:OP1 | 2.14 | 0.48 |
| 25:YA:2146:C:H4' | 25:YA:2147:G:C8 | 2.48 | 0.48 |
| 25:YA:2364:C:H2' | 25:YA:2365:G:O4' | 2.13 | 0.48 |
| 25:YA:2528:U:H2' | 25:YA:2530:A:O5' | 2.14 | 0.48 |
| 25:YA:2816:C:O2 | 25:YA:2883:A:O2' | 2.26 | 0.48 |
| 25:YA:2745:C:O2' | 31:YH:139:GLN:HA | 2.14 | 0.48 |
| 44:YY:9:LYS:HE2 | 44:YY:28:LYS:O | 2.13 | 0.48 |
| 1:QA:1301:U:O2' | 1:QA:1302:U:OP1 | 2.32 | 0.47 |
| 1:QA:570:G:H2' | 1:QA:571:U:C6 | 2.49 | 0.47 |
| 25:RA:579:G:H2' | 25:RA:580:C:C6 | 2.49 | 0.47 |
| 25:RA:953:A:OP2 | 36:RQ:16:ARG:HD3 | 2.14 | 0.47 |
| 25:RA:1423:G:H5'' | 27:RD:33:LEU:HD11 | 1.96 | 0.47 |
| 29:RF:125:LEU:HA | 29:RF:194:MET:O | 2.14 | 0.47 |
| 36:RQ:19:GLY:O | 36:RQ:98:LYS:HD3 | 2.13 | 0.47 |
| 1:XA:389:A:H3' | 1:XA:390:C:C6 | 2.48 | 0.47 |
| 1:XA:481:G:O2' | 1:XA:482:A:O5' | 2.32 | 0.47 |
| 1:XA:946:A:H2' | 1:XA:947:G:H8 | 1.79 | 0.47 |
| 11:XK:110:ASP:HB2 | 18:XR:88:LYS:HD2 | 1.95 | 0.47 |
| 20:XT:20:LEU:O | 20:XT:23:ARG:HG2 | 2.14 | 0.47 |
| 25:YA:1204:A:H1' | 25:YA:1206:G:C8 | 2.49 | 0.47 |
| 25:YA:1290:C:H2' | 25:YA:1291:C:H6 | 1.79 | 0.47 |
| 25:YA:2547:U:H2' | 25:YA:2548:G:H8 | 1.79 | 0.47 |
| 25:YA:2646:C:H2' | 25:YA:2647:U:O4' | 2.14 | 0.47 |
| 25:YA:458:G:N2 | 25:YA:470:A:OP2 | 2.47 | 0.47 |
| 25:YA:764:A:H5' | 27:YD:210:GLY:HA2 | 1.96 | 0.47 |
| 26:YB:32:C:N3 | 26:YB:51:G:N2 | 2.62 | 0.47 |
| 30:YG:37:VAL:HG22 | 30:YG:159:VAL:HG12 | 1.95 | 0.47 |
| 35:YP:84:ASN:HA | 35:YP:115:LEU:O | 2.15 | 0.47 |
| 45:YZ:182:LYS:O | 45:YZ:182:LYS:HD3 | 2.14 | 0.47 |
| 1:QA:246:A:C2 | 1:QA:282:A:C5 | 3.02 | 0.47 |
| 1:QA:260:G:H2' | 1:QA:261:U:C6 | 2.49 | 0.47 |
| 1:QA:667:G:H2' | 1:QA:668:G:C8 | 2.49 | 0.47 |
| 4:QD:155:LEU:O | 4:QD:158:ILE:N | 2.47 | 0.47 |
| 13:QM:14:ARG:NH1 | 13:QM:42:ALA:HA | 2.28 | 0.47 |
| 26:RB:11:C:OP1 | 46:R0:72:ARG:NE | 2.47 | 0.47 |
| 25:RA:570:G:H2' | 25:RA:2030:A:C6 | 2.48 | 0.47 |
| 25:RA:2836:U:H2' | 25:RA:2837:G:H8 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2859:G:H2' | 25:RA:2860:A:C8 | 2.49 | 0.47 |
| 25:RA:181:A:H1' | 25:RA:435:C:H5' | 1.96 | 0.47 |
| 25:RA:65:C:O2' | 25:RA:456:C:N3 | 2.46 | 0.47 |
| 34:RO:8:LEU:HB2 | 34:RO:19:ILE:HG13 | 1.96 | 0.47 |
| 1:XA:1384:C:H2' | 1:XA:1385:G:H8 | 1.80 | 0.47 |
| 1:XA:1422:G:H2' | 1:XA:1423:G:H8 | 1.78 | 0.47 |
| 1:XA:1486:G:H2' | 1:XA:1487:G:C8 | 2.49 | 0.47 |
| 1:XA:1518:A:H2' | 1:XA:1519:A:C8 | 2.48 | 0.47 |
| 1:XA:412:A:H4' | 1:XA:413:G:O5' | 2.13 | 0.47 |
| 2:XB:69:LEU:HB3 | 2:XB:162:ILE:HG22 | 1.95 | 0.47 |
| 2:XB:205:ASP:OD1 | 2:XB:206:ASP:N | 2.46 | 0.47 |
| 1:XA:707:C:H4' | 11:XK:20:TYR:CD2 | 2.49 | 0.47 |
| 13:XM:117:VAL:HG22 | 13:XM:118:ALA:H | 1.79 | 0.47 |
| 14:YN:4:LYS:HA | 14:YN:7:ILE:HG12 | 1.96 | 0.47 |
| 25:YA:2755:C:C4 | 55:Y9:1:MET:HG2 | 2.47 | 0.47 |
| 31:YH:145:ALA:C | 55:Y9:20:HIS:CD2 | 2.87 | 0.47 |
| 25:YA:1210:A:H4' | 25:YA:1211:U:O5' | 2.14 | 0.47 |
| 25:YA:1399:C:H2' | 25:YA:1400:G:C8 | 2.48 | 0.47 |
| 25:YA:1429:G:H2' | 25:YA:1430:C:C6 | 2.49 | 0.47 |
| 25:YA:1475:G:H2' | 25:YA:1476:C:C6 | 2.49 | 0.47 |
| 25:YA:2740:A:C2 | 25:YA:2741:A:C6 | 3.02 | 0.47 |
| 25:YA:603:A:N1 | 25:YA:625:G:O2' | 2.44 | 0.47 |
| 25:YA:971:C:H2' | 25:YA:972:G:O4' | 2.13 | 0.47 |
| 26:YB:31:C:N4 | 26:YB:51:G:H1 | 2.12 | 0.47 |
| 28:YE:104:VAL:HG11 | 28:YE:188:VAL:HG23 | 1.96 | 0.47 |
| 31:YH:121:ILE:HG13 | 31:YH:144:VAL:HG21 | 1.97 | 0.47 |
| 38:YS:66:ALA:HA | 38:YS:69:VAL:HG12 | 1.95 | 0.47 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:H8 | 1.78 | 0.47 |
| 1:QA:1112:C:H1' | 3:QC:179:ARG:HH11 | 1.79 | 0.47 |
| 1:QA:1264:C:H2' | 1:QA:1265:G:C8 | 2.49 | 0.47 |
| 1:QA:1354:C:H2' | 1:QA:1355:G:H8 | 1.79 | 0.47 |
| 10:QJ:13:HIS:HB3 | 10:QJ:68:HIS:CD2 | 2.49 | 0.47 |
| 20:QT:29:LYS:O | 20:QT:33:ILE:HG12 | 2.14 | 0.47 |
| 20:QT:90:GLN:O | 20:QT:93:GLU:HG2 | 2.14 | 0.47 |
| 22:QW:9:G:H5" | 22:QW:10:G:OP2 | 2.15 | 0.47 |
| 48:R2:10:LEU:HD21 | 48:R2:59:ARG:HD2 | 1.97 | 0.47 |
| 49:R3:15:TYR:CE2 | 49:R3:53:LEU:HD21 | 2.47 | 0.47 |
| 25:RA:2292:C:H2' | 25:RA:2293:C:H6 | 1.80 | 0.47 |
| 25:RA:575:A:OP2 | 25:RA:2499:C:O2' | 2.27 | 0.47 |
| 27:RD:35:LYS:NZ | 27:RD:64:ILE:O | 2.44 | 0.47 |
| 39:RT:53:ARG:O | 39:RT:59:THR:HG23 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1425:U:H2' | 1:XA:1426:C:C6 | 2.49 | 0.47 |
| 1:XA:196:A:OP1 | 20:XT:68:LYS:NZ | 2.35 | 0.47 |
| 1:XA:34:C:H2' | 1:XA:35:G:C8 | 2.48 | 0.47 |
| 8:XH:20:TYR:CE2 | 8:XH:75:ARG:HD2 | 2.49 | 0.47 |
| 15:XO:15:PHE:HD2 | 15:XO:30:ALA:HB2 | 1.78 | 0.47 |
| 25:YA:1338:G:N7 | 43:YX:62:LYS:NZ | 2.50 | 0.47 |
| 25:YA:1430:C:H2' | 25:YA:1431:U:H6 | 1.76 | 0.47 |
| 25:YA:2233:U:H2' | 25:YA:2234:G:C8 | 2.49 | 0.47 |
| 25:YA:2648:C:H2' | 25:YA:2649:U:H6 | 1.79 | 0.47 |
| 25:YA:1662:C:H1' | 25:YA:2687:U:H5'' | 1.97 | 0.47 |
| 25:YA:26:G:O2' | 25:YA:514:A:N6 | 2.44 | 0.47 |
| 25:YA:690:G:H2' | 25:YA:691:C:C6 | 2.48 | 0.47 |
| 1:QA:1159:U:O2' | 1:QA:1181:G:N2 | 2.45 | 0.47 |
| 1:QA:295:C:H2' | 1:QA:296:U:O4' | 2.14 | 0.47 |
| 1:QA:370:C:H2' | 1:QA:371:G:H8 | 1.78 | 0.47 |
| 1:QA:867:G:HO2' | 1:QA:873:A:N6 | 2.12 | 0.47 |
| 8:QH:104:ARG:HD2 | 8:QH:138:TRP:CD2 | 2.50 | 0.47 |
| 12:QL:30:ALA:HB3 | 12:QL:33:ARG:HD3 | 1.95 | 0.47 |
| 13:QM:58:GLU:O | 13:QM:62:ASN:HB2 | 2.13 | 0.47 |
| 49:R3:6:VAL:HB | 49:R3:54:VAL:HG21 | 1.95 | 0.47 |
| 55:R9:14:CYS:HA | 55:R9:27:CYS:SG | 2.54 | 0.47 |
| 25:RA:1291:C:H2' | 25:RA:1292:U:H6 | 1.80 | 0.47 |
| 25:RA:1709:U:H2' | 25:RA:1710:C:H6 | 1.78 | 0.47 |
| 25:RA:2443:C:H2' | 25:RA:2444:G:H8 | 1.79 | 0.47 |
| 25:RA:2455:G:H2' | 25:RA:2456:C:C6 | 2.50 | 0.47 |
| 25:RA:39:C:H2' | 25:RA:40:C:C6 | 2.49 | 0.47 |
| 25:RA:968:G:H2' | 25:RA:969:U:C6 | 2.49 | 0.47 |
| 29:RF:198:ALA:HA | 29:RF:201:VAL:HG12 | 1.96 | 0.47 |
| 41:RV:22:VAL:HG12 | 41:RV:23:GLU:H | 1.78 | 0.47 |
| 45:RZ:94:GLU:HB2 | 45:RZ:95:PRO:HD3 | 1.95 | 0.47 |
| 1:XA:739:C:O2' | 15:XO:42:HIS:ND1 | 2.47 | 0.47 |
| 25:YA:1216:G:OP1 | 40:YU:11:ARG:NH2 | 2.36 | 0.47 |
| 25:YA:1539:G:H2' | 25:YA:1540:G:H8 | 1.79 | 0.47 |
| 25:YA:1562:A:H2' | 25:YA:1563:G:C8 | 2.49 | 0.47 |
| 25:YA:2047:U:H2' | 25:YA:2048:G:H8 | 1.77 | 0.47 |
| 25:YA:2752:C:C4 | 25:YA:2753:A:C6 | 3.02 | 0.47 |
| 25:YA:64:A:O3' | 43:YX:71:GLY:HA3 | 2.15 | 0.47 |
| 25:YA:949:C:H2' | 25:YA:950:G:C8 | 2.50 | 0.47 |
| 34:YO:2:ILE:N | 34:YO:33:ALA:O | 2.43 | 0.47 |
| 45:YZ:112:ARG:HG3 | 45:YZ:113:ALA:N | 2.29 | 0.47 |
| 1:QA:420:U:N3 | 1:QA:422:C:O2 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:436:C:H2' | 1:QA:437:U:H6 | 1.78 | 0.47 |
| 22:QV:24:C:H2' | 22:QV:25:U:H6 | 1.78 | 0.47 |
| 22:QV:35:C:H2' | 22:QV:36:A:C8 | 2.48 | 0.47 |
| 22:QV:53:G:O2' | 22:QV:54:G:OP1 | 2.29 | 0.47 |
| 25:RA:1265:A:OP1 | 25:RA:1265:A:H8 | 1.97 | 0.47 |
| 25:RA:2131:G:H4' | 25:RA:2132:U:H4' | 1.95 | 0.47 |
| 25:RA:2643:G:H2' | 25:RA:2644:G:O4' | 2.14 | 0.47 |
| 25:RA:593:G:H2' | 25:RA:594:U:C6 | 2.50 | 0.47 |
| 25:RA:598:G:C4' | 35:RP:11:GLY:HA3 | 2.44 | 0.47 |
| 31:RH:12:PRO:HG3 | 31:RH:48:GLY:HA2 | 1.96 | 0.47 |
| 45:RZ:68:PRO:HG2 | 45:RZ:91:LEU:HB2 | 1.96 | 0.47 |
| 1:XA:1308:U:H2' | 1:XA:1309:G:C8 | 2.48 | 0.47 |
| 1:XA:1507:A:H2' | 1:XA:1508:G:C8 | 2.49 | 0.47 |
| 1:XA:501:C:H1' | 1:XA:549:C:H1' | 1.96 | 0.47 |
| 1:XA:807:A:H2' | 1:XA:808:C:C6 | 2.50 | 0.47 |
| 9:XI:114:TYR:HE2 | 10:XJ:59:SER:HA | 1.80 | 0.47 |
| 25:YA:2080:G:H5' | 47:Y1:19:GLN:HG3 | 1.96 | 0.47 |
| 25:YA:49:A:N7 | 25:YA:120:U:H5 | 2.12 | 0.47 |
| 25:YA:691:C:H2' | 25:YA:692:C:H6 | 1.78 | 0.47 |
| 25:YA:752:A:H4' | 25:YA:753:C:O5' | 2.14 | 0.47 |
| 30:YG:125:PHE:CE2 | 30:YG:170:ARG:HB2 | 2.48 | 0.47 |
| 30:YG:95:ARG:O | 30:YG:99:MET:HG2 | 2.14 | 0.47 |
| 1:QA:359:U:OP1 | 32:YI:87:LYS:NZ | 2.45 | 0.47 |
| 1:QA:690:G:H2' | 1:QA:691:G:O4' | 2.15 | 0.47 |
| 1:QA:861:G:O6 | 1:QA:869:G:N2 | 2.47 | 0.47 |
| 2:QB:237:ALA:O | 2:QB:239:VAL:N | 2.47 | 0.47 |
| 14:QN:4:LYS:HA | 14:QN:7:ILE:HG12 | 1.95 | 0.47 |
| 16:QP:18:ARG:HA | 16:QP:38:TYR:HA | 1.97 | 0.47 |
| 25:RA:2212:A:H1' | 25:RA:2215:G:C5 | 2.50 | 0.47 |
| 25:RA:2542:A:H5' | 25:RA:2543:G:OP1 | 2.13 | 0.47 |
| 25:RA:270(Y):G:H2' | 25:RA:270(Z):U:C6 | 2.50 | 0.47 |
| 25:RA:439:G:H2' | 25:RA:440:G:H8 | 1.79 | 0.47 |
| 25:RA:639:U:H2' | 25:RA:640:C:C6 | 2.50 | 0.47 |
| 25:RA:729:G:O2' | 25:RA:763:G:H4' | 2.14 | 0.47 |
| 27:RD:77:ALA:HB3 | 27:RD:117:VAL:HG13 | 1.97 | 0.47 |
| 35:RP:63:PRO:HB3 | 54:R8:13:ARG:HB3 | 1.95 | 0.47 |
| 36:RQ:66:ILE:HA | 36:RQ:104:PHE:HD1 | 1.80 | 0.47 |
| 44:RY:20:TYR:CE2 | 44:RY:43:ASN:HA | 2.49 | 0.47 |
| 45:RZ:150:LEU:HB2 | 45:RZ:154:ASP:OD2 | 2.15 | 0.47 |
| 1:XA:1095:U:H5'' | 1:XA:1109:C:O2 | 2.15 | 0.47 |
| 1:XA:1327:C:H2' | 1:XA:1328:C:H6 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:1446:A:H5' | 39:YT:122:ASP:OD1 | 2.15 | 0.47 |
| 1:XA:177:C:H2' | 1:XA:178:C:H6 | 1.80 | 0.47 |
| 1:XA:868:C:H2' | 1:XA:869:G:O4' | 2.13 | 0.47 |
| 1:XA:891:U:H2' | 1:XA:892:A:H8 | 1.80 | 0.47 |
| 3:XC:43:LEU:O | 3:XC:47:LEU:HB2 | 2.15 | 0.47 |
| 5:XE:99:GLY:N | 5:XE:117:ASP:OD1 | 2.41 | 0.47 |
| 8:XH:104:ARG:HD2 | 8:XH:138:TRP:CD2 | 2.49 | 0.47 |
| 49:Y3:6:VAL:HG12 | 49:Y3:56:VAL:HG22 | 1.96 | 0.47 |
| 25:YA:141:A:C8 | 25:YA:1408:C:H1' | 2.49 | 0.47 |
| 25:YA:1535:U:N3 | 25:YA:1537:C:H1' | 2.30 | 0.47 |
| 25:YA:1590:U:H2' | 25:YA:1591:G:C8 | 2.48 | 0.47 |
| 25:YA:1729:A:H2' | 25:YA:1730:U:H5'' | 1.96 | 0.47 |
| 25:YA:24:G:C6 | 25:YA:25:U:C4 | 3.02 | 0.47 |
| 25:YA:27:G:H1' | 25:YA:513:A:H62 | 1.79 | 0.47 |
| 25:YA:2853:C:H2' | 25:YA:2854:G:C8 | 2.48 | 0.47 |
| 27:YD:153:ALA:O | 27:YD:157:ARG:NH1 | 2.47 | 0.47 |
| 25:YA:2851:A:O2' | 37:YR:64:ARG:NH2 | 2.47 | 0.47 |
| 1:QA:1288:A:N1 | 1:QA:1371:G:H1' | 2.30 | 0.47 |
| 1:QA:481:G:O2' | 1:QA:482:A:O5' | 2.33 | 0.47 |
| 1:QA:503:C:OP2 | 12:QL:116:SER:OG | 2.24 | 0.47 |
| 1:QA:687:A:N6 | 1:QA:703:G:C2 | 2.82 | 0.47 |
| 7:QG:111:ARG:HG2 | 7:QG:113:GLU:OE1 | 2.14 | 0.47 |
| 7:QG:15:ASP:HB3 | 7:QG:19:GLY:H | 1.79 | 0.47 |
| 7:QG:69:VAL:HG21 | 7:QG:104:LEU:HD21 | 1.97 | 0.47 |
| 46:R0:53:MET:HB3 | 46:R0:59:LEU:HD23 | 1.96 | 0.47 |
| 55:R9:24:TYR:CE1 | 55:R9:35:ARG:HG3 | 2.50 | 0.47 |
| 25:RA:270(V):G:H2' | 25:RA:270(W):G:H8 | 1.80 | 0.47 |
| 45:RZ:40:ASP:HB3 | 45:RZ:43:GLU:HB2 | 1.95 | 0.47 |
| 1:XA:1028(B):C:N4 | 1:XA:1029:G:H1' | 2.30 | 0.47 |
| 1:XA:1443:G:H5' | 1:XA:1446:A:OP2 | 2.14 | 0.47 |
| 1:XA:664:G:H22 | 1:XA:741:G:H1 | 1.63 | 0.47 |
| 1:XA:921:U:O2 | 5:XE:19:MET:HB2 | 2.15 | 0.47 |
| 11:XK:27:ASN:OD1 | 11:XK:28:THR:N | 2.47 | 0.47 |
| 1:XA:227:G:N2 | 16:XP:62:VAL:O | 2.41 | 0.47 |
| 46:Y0:32:ARG:N | 46:Y0:35:ASN:OD1 | 2.42 | 0.47 |
| 25:YA:2059:A:H5' | 25:YA:2060:A:OP2 | 2.15 | 0.47 |
| 25:YA:740:U:H2' | 25:YA:741:G:C8 | 2.50 | 0.47 |
| 32:YI:14:ASP:O | 32:YI:16:GLY:N | 2.45 | 0.47 |
| 34:YO:107:ARG:NH1 | 39:YT:36:GLU:OE1 | 2.48 | 0.47 |
| 41:YV:22:VAL:HG12 | 41:YV:23:GLU:H | 1.79 | 0.47 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C4 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1300:G:H1' | 1:QA:1303:C:H42 | 1.80 | 0.47 |
| 1:QA:1525:G:H2' | 1:QA:1526:G:H8 | 1.79 | 0.47 |
| 1:QA:20:U:H2' | 1:QA:21:G:O4' | 2.14 | 0.47 |
| 1:QA:575:G:O2' | 1:QA:821:G:H5' | 2.14 | 0.47 |
| 7:QG:46:ALA:O | 7:QG:50:ILE:HG12 | 2.15 | 0.47 |
| 1:QA:1255:G:OP2 | 10:QJ:45:ARG:NH2 | 2.47 | 0.47 |
| 13:QM:117:VAL:HG22 | 13:QM:118:ALA:H | 1.79 | 0.47 |
| 22:QV:35:C:O2' | 22:QV:36:A:OP1 | 2.26 | 0.47 |
| 22:QW:2:G:H2' | 22:QW:3:C:C6 | 2.50 | 0.47 |
| 25:RA:1032:A:O2' | 25:RA:1033:U:OP1 | 2.27 | 0.47 |
| 25:RA:2025:C:H2' | 25:RA:2026:C:C6 | 2.50 | 0.47 |
| 25:RA:2680:C:H5' | 28:RE:189:PRO:HA | 1.96 | 0.47 |
| 25:RA:274:G:H2' | 25:RA:275:G:O4' | 2.15 | 0.47 |
| 25:RA:776:G:N7 | 25:RA:793:A:O2' | 2.48 | 0.47 |
| 27:RD:201:HIS:O | 27:RD:204:ILE:HG12 | 2.14 | 0.47 |
| 29:RF:184:TYR:CE2 | 29:RF:188:ARG:HD2 | 2.50 | 0.47 |
| 30:RG:41:GLN:HE21 | 30:RG:153:ARG:HB3 | 1.80 | 0.47 |
| 25:RA:1155:A:OP1 | 40:RU:55:ARG:HD2 | 2.15 | 0.47 |
| 41:RV:4:ILE:HG13 | 41:RV:40:LEU:HD12 | 1.96 | 0.47 |
| 25:RA:1266:G:N7 | 42:RW:15:ARG:HD2 | 2.30 | 0.47 |
| 25:RA:483:A:O2' | 44:RY:49:VAL:O | 2.24 | 0.47 |
| 1:XA:299:A:H2' | 1:XA:300:A:C8 | 2.50 | 0.47 |
| 1:XA:728:A:H2' | 1:XA:729:A:C8 | 2.49 | 0.47 |
| 6:XF:12:PRO:HD3 | 6:XF:58:GLY:HA2 | 1.97 | 0.47 |
| 7:XG:22:LEU:HG | 7:XG:62:PHE:HE2 | 1.79 | 0.47 |
| 25:YA:1191:G:H2' | 25:YA:1192:G:O4' | 2.15 | 0.47 |
| 25:YA:1505:C:H2' | 25:YA:1506:C:C6 | 2.49 | 0.47 |
| 25:YA:1689:A:H2' | 25:YA:1690:A:C8 | 2.49 | 0.47 |
| 25:YA:2416:C:C2 | 25:YA:2417:C:C5 | 3.03 | 0.47 |
| 25:YA:273(C):C:H2' | 25:YA:273(D):C:H6 | 1.80 | 0.47 |
| 25:YA:533:G:N2 | 40:YU:49:HIS:HE1 | 2.13 | 0.47 |
| 29:YF:34:TRP:CE3 | 35:YP:8:PRO:HB3 | 2.49 | 0.47 |
| 30:YG:32:PRO:HB3 | 30:YG:163:ALA:HB2 | 1.97 | 0.47 |
| 40:YU:92:ARG:HB2 | 41:YV:11:GLN:OE1 | 2.15 | 0.47 |
| 1:QA:1223:C:P | 1:QA:1224:G:H2' | 2.55 | 0.47 |
| 1:QA:1250:A:H2 | 1:QA:1370:G:H1' | 1.80 | 0.47 |
| 1:QA:152:A:H62 | 1:QA:169:C:H42 | 1.63 | 0.47 |
| 1:QA:538:G:H2' | 1:QA:539:A:H8 | 1.80 | 0.47 |
| 1:QA:948:C:H2' | 1:QA:949:A:H8 | 1.79 | 0.47 |
| 1:QA:1192:C:P | 3:QC:4:LYS:HZ1 | 2.35 | 0.47 |
| 1:QA:35:G:O2' | 12:QL:118:SER:O | 2.26 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:1482:U:H5' | 25:RA:1483:G:OP2 | 2.15 | 0.47 |
| 25:RA:310:A:H1' | 25:RA:311:A:H2' | 1.97 | 0.47 |
| 25:RA:389:G:H1 | 35:RP:70:GLN:HB3 | 1.80 | 0.47 |
| 25:RA:598:G:O2' | 35:RP:9:ASN:ND2 | 2.43 | 0.47 |
| 25:RA:635:C:O2' | 25:RA:639:U:OP1 | 2.33 | 0.47 |
| 27:RD:122:ASP:OD1 | 27:RD:123:ALA:N | 2.43 | 0.47 |
| 25:RA:321:G:OP2 | 29:RF:135:LYS:HD3 | 2.15 | 0.47 |
| 33:RN:12:ARG:NH1 | 33:RN:14:VAL:HG22 | 2.29 | 0.47 |
| 34:RO:78:ARG:HH21 | 39:RT:103:ARG:NH2 | 2.13 | 0.47 |
| 38:RS:110:LEU:O | 38:RS:112:PHE:HD1 | 1.98 | 0.47 |
| 1:XA:1227:A:OP2 | 13:XM:111:LYS:HE3 | 2.15 | 0.47 |
| 2:XB:93:VAL:HG11 | 2:XB:97:TRP:HD1 | 1.80 | 0.47 |
| 1:XA:27:G:H5' | 4:XD:209:ARG:HE | 1.80 | 0.47 |
| 21:XU:6:ARG:HE | 21:XU:15:ARG:HH21 | 1.63 | 0.47 |
| 25:YA:208:C:H2' | 25:YA:209:C:C6 | 2.49 | 0.47 |
| 25:YA:373:U:H1' | 25:YA:423:A:N3 | 2.30 | 0.47 |
| 25:YA:960:A:C8 | 25:YA:962:G:C8 | 3.03 | 0.47 |
| 25:YA:598:G:O3' | 35:YP:9:ASN:ND2 | 2.48 | 0.47 |
| 1:QA:1160:G:H1 | 1:QA:1177:G:N2 | 2.12 | 0.47 |
| 1:QA:46:G:O2' | 1:QA:365:U:O2' | 2.14 | 0.47 |
| 1:QA:439:A:OP2 | 1:QA:493:G:N1 | 2.48 | 0.47 |
| 5:QE:35:GLY:HA3 | 5:QE:112:LEU:HB3 | 1.97 | 0.47 |
| 13:QM:92:HIS:CD2 | 13:QM:98:VAL:HG21 | 2.50 | 0.47 |
| 25:RA:1070:A:N7 | 25:RA:1096:A:H2' | 2.30 | 0.47 |
| 25:RA:1157:G:O2' | 49:R3:31:LEU:HD12 | 2.15 | 0.47 |
| 25:RA:2581:G:OP2 | 25:RA:2581:G:N2 | 2.48 | 0.47 |
| 25:RA:2870:C:H2' | 25:RA:2871:C:O4' | 2.14 | 0.47 |
| 25:RA:640:C:H2' | 25:RA:641:C:C6 | 2.50 | 0.47 |
| 26:RB:60:C:H2' | 26:RB:61:G:H8 | 1.80 | 0.47 |
| 33:RN:95:PRO:C | 33:RN:97:ARG:H | 2.17 | 0.47 |
| 34:RO:76:ALA:HB3 | 39:RT:75:ILE:HD12 | 1.97 | 0.47 |
| 41:RV:5:VAL:HG11 | 41:RV:57:VAL:HG21 | 1.97 | 0.47 |
| 1:XA:1287:A:C2 | 1:XA:1353:G:H1' | 2.48 | 0.47 |
| 1:XA:1321:C:OP2 | 1:XA:1322:C:H2' | 2.15 | 0.47 |
| 1:XA:636:U:H5' | 17:XQ:2:PRO:HG3 | 1.97 | 0.47 |
| 1:XA:739:C:HO2' | 15:XO:42:HIS:HD1 | 1.59 | 0.47 |
| 2:XB:30:ARG:H | 2:XB:30:ARG:HD3 | 1.79 | 0.47 |
| 1:XA:1348:U:H4' | 9:XI:120:ARG:HD2 | 1.96 | 0.47 |
| 13:XM:83:ASP:H | 13:XM:93:ARG:HH21 | 1.62 | 0.47 |
| 25:YA:2577:A:H5' | 51:Y5:3:LYS:NZ | 2.30 | 0.47 |
| 25:YA:86:C:H4' | 25:YA:104:U:H1' | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:1062:G:H2' | 25:YA:1063:G:C8 | 2.49 | 0.47 |
| 25:YA:1290:C:H2' | 25:YA:1291:C:C6 | 2.50 | 0.47 |
| 25:YA:1689:A:OP2 | 25:YA:1698:A:N6 | 2.43 | 0.47 |
| 25:YA:2359:C:H2' | 25:YA:2360:A:O4' | 2.15 | 0.47 |
| 25:YA:375:C:H2' | 25:YA:376:C:H6 | 1.80 | 0.47 |
| 25:YA:579:G:H2' | 25:YA:580:C:C6 | 2.50 | 0.47 |
| 25:YA:2746:U:H4' | 31:YH:138:LYS:HD3 | 1.96 | 0.47 |
| 39:YT:25:GLY:H | 39:YT:49:VAL:HG13 | 1.78 | 0.47 |
| 40:YU:21:ALA:HA | 40:YU:24:TYR:CE2 | 2.49 | 0.47 |
| 1:QA:1160:G:N3 | 1:QA:1160:G:H2' | 2.30 | 0.47 |
| 1:QA:1305:G:O2' | 1:QA:1306:A:H8 | 1.97 | 0.47 |
| 1:QA:560:U:H5' | 1:QA:566:G:N2 | 2.30 | 0.47 |
| 1:QA:946:A:H2' | 1:QA:947:G:H8 | 1.80 | 0.47 |
| 1:QA:978:A:C4 | 1:QA:1319:A:C2 | 3.03 | 0.47 |
| 4:QD:173:TRP:CD1 | 4:QD:174:LEU:HG | 2.50 | 0.47 |
| 11:QK:91:ARG:O | 11:QK:95:ILE:HG12 | 2.15 | 0.47 |
| 1:QA:1216:G:H5'' | 14:QN:5:ALA:HB2 | 1.95 | 0.47 |
| 17:QQ:51:TYR:HE2 | 17:QQ:73:VAL:HG11 | 1.79 | 0.47 |
| 19:QS:67:VAL:HG11 | 50:R4:58:ARG:O | 2.15 | 0.47 |
| 25:RA:191:A:H2' | 25:RA:192:C:C6 | 2.49 | 0.47 |
| 25:RA:2626:C:H2' | 25:RA:2627:G:H8 | 1.80 | 0.47 |
| 25:RA:299:A:N3 | 25:RA:319:C:O2' | 2.42 | 0.47 |
| 27:RD:244:ARG:HB2 | 27:RD:245:PRO:HD2 | 1.96 | 0.47 |
| 27:RD:93:ALA:HB2 | 27:RD:107:ALA:HB2 | 1.96 | 0.47 |
| 31:RH:149:ARG:NH2 | 31:RH:164:TYR:OH | 2.47 | 0.47 |
| 40:RU:90:VAL:HG12 | 40:RU:91:ASP:N | 2.29 | 0.47 |
| 45:RZ:112:ARG:HG3 | 45:RZ:113:ALA:N | 2.30 | 0.47 |
| 1:XA:1386:G:H2' | 1:XA:1387:G:H8 | 1.80 | 0.47 |
| 1:XA:320:C:H2' | 1:XA:321:A:C8 | 2.50 | 0.47 |
| 1:XA:369:C:OP2 | 1:XA:388:G:N2 | 2.47 | 0.47 |
| 1:XA:452:A:H2' | 1:XA:453:A:O4' | 2.14 | 0.47 |
| 1:XA:600:C:H5' | 8:XH:129:VAL:O | 2.15 | 0.47 |
| 1:XA:986:A:H2' | 1:XA:987:G:C8 | 2.50 | 0.47 |
| 1:XA:1108:G:H5' | 3:XC:176:HIS:HD2 | 1.80 | 0.47 |
| 4:XD:166:LYS:HB2 | 4:XD:178:VAL:HG11 | 1.96 | 0.47 |
| 6:XF:67:MET:HB2 | 6:XF:68:PRO:HD2 | 1.97 | 0.47 |
| 1:XA:186:C:O2' | 20:XT:85:MET:SD | 2.63 | 0.47 |
| 22:XW:32:G:H3' | 22:XW:33:C:O4' | 2.15 | 0.47 |
| 22:XW:49:C:N3 | 22:XW:60:A:H1' | 2.29 | 0.47 |
| 49:Y3:15:TYR:HE2 | 49:Y3:53:LEU:HD21 | 1.80 | 0.47 |
| 25:YA:1520:U:H2' | 25:YA:1521:G:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1899:G:H21 | 25:YA:1902:C:N4 | 2.13 | 0.47 |
| 25:YA:2564:A:C6 | 25:YA:2647:U:H4' | 2.49 | 0.47 |
| 25:YA:270(G):C:H2' | 25:YA:270(H):C:C6 | 2.50 | 0.47 |
| 25:YA:2756:U:C4 | 25:YA:2759:G:C8 | 3.02 | 0.47 |
| 25:YA:643:A:N1 | 25:YA:2369:A:O2' | 2.37 | 0.47 |
| 26:YB:22:U:H3 | 26:YB:61:G:H1 | 1.63 | 0.47 |
| 27:YD:31:LYS:HE3 | 27:YD:102:LYS:HD3 | 1.95 | 0.47 |
| 27:YD:79:VAL:HA | 27:YD:95:LEU:HD23 | 1.97 | 0.47 |
| 25:YA:2635:C:H5'' | 28:YE:78:LEU:HA | 1.96 | 0.47 |
| 39:YT:120:ARG:HA | 39:YT:123:GLN:HB2 | 1.95 | 0.47 |
| 1:QA:1124:G:H3' | 1:QA:1145:C:N4 | 2.30 | 0.46 |
| 1:QA:1486:G:H2' | 1:QA:1487:G:C8 | 2.49 | 0.46 |
| 1:QA:328:C:H1' | 1:QA:329:A:OP2 | 2.15 | 0.46 |
| 1:QA:790:A:H2' | 1:QA:791:G:C8 | 2.50 | 0.46 |
| 1:QA:970:C:H42 | 9:QL:128:ARG:C | 2.18 | 0.46 |
| 10:QJ:28:ARG:NH2 | 10:QJ:34:VAL:O | 2.48 | 0.46 |
| 10:QJ:78:ASN:O | 10:QJ:81:THR:OG1 | 2.26 | 0.46 |
| 1:QA:674:G:H1' | 18:QR:81:PHE:HE2 | 1.80 | 0.46 |
| 25:RA:839:U:H1' | 25:RA:1191:G:H1' | 1.96 | 0.46 |
| 25:RA:2251:G:C8 | 25:RA:2450:A:H4' | 2.50 | 0.46 |
| 25:RA:2685:G:P | 39:RT:51:ARG:HH22 | 2.38 | 0.46 |
| 25:RA:2697:G:H2' | 25:RA:2698:U:C6 | 2.50 | 0.46 |
| 31:RH:120:GLY:HA3 | 31:RH:140:LYS:NZ | 2.30 | 0.46 |
| 25:RA:559:G:H22 | 40:RU:49:HIS:CE1 | 2.33 | 0.46 |
| 45:RZ:99:TYR:CE1 | 45:RZ:125:LEU:HB2 | 2.50 | 0.46 |
| 1:XA:335:C:H2' | 1:XA:336:C:C6 | 2.50 | 0.46 |
| 1:XA:363:A:C2 | 12:XL:31:PRO:HD2 | 2.50 | 0.46 |
| 1:XA:422:C:O2' | 1:XA:423:G:N2 | 2.49 | 0.46 |
| 13:XM:16:ASP:OD1 | 13:XM:17:VAL:N | 2.45 | 0.46 |
| 18:XR:51:LEU:HD22 | 18:XR:55:ARG:HD2 | 1.97 | 0.46 |
| 46:Y0:46:LYS:HD2 | 46:Y0:78:TYR:HE1 | 1.79 | 0.46 |
| 49:Y3:15:TYR:O | 49:Y3:20:LYS:NZ | 2.48 | 0.46 |
| 25:YA:1478:G:H1' | 25:YA:1557:C:O2' | 2.15 | 0.46 |
| 25:YA:1539:G:H2' | 25:YA:1540:G:C8 | 2.50 | 0.46 |
| 25:YA:2212:A:H1' | 25:YA:2215:G:C5 | 2.51 | 0.46 |
| 25:YA:247:G:H4' | 25:YA:386:G:C5 | 2.50 | 0.46 |
| 25:YA:2665:A:H2' | 25:YA:2666:C:O4' | 2.14 | 0.46 |
| 25:YA:638:G:H2' | 25:YA:639:U:C6 | 2.50 | 0.46 |
| 25:YA:87:C:H5'' | 25:YA:88:G:H5' | 1.97 | 0.46 |
| 25:YA:1257:C:H4' | 29:YF:83:PHE:CE1 | 2.49 | 0.46 |
| 33:YN:22:THR:HA | 33:YN:61:ARG:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:YO:23:ARG:NH2 | 34:YO:28:SER:O | 2.47 | 0.46 |
| 38:YS:34:HIS:CE1 | 38:YS:54:LEU:HD12 | 2.50 | 0.46 |
| 42:YW:111:HIS:HD2 | 42:YW:113:LYS:H | 1.62 | 0.46 |
| 1:QA:1066:C:H3' | 1:QA:1067:A:H8 | 1.81 | 0.46 |
| 1:QA:401:C:H2' | 1:QA:402:G:H8 | 1.80 | 0.46 |
| 1:QA:771:G:H2' | 1:QA:772:U:C6 | 2.50 | 0.46 |
| 1:QA:877:C:H2' | 1:QA:878:G:H8 | 1.80 | 0.46 |
| 6:QF:21:LEU:O | 6:QF:25:ILE:HG12 | 2.14 | 0.46 |
| 9:QI:22:GLY:HA3 | 9:QI:60:ASP:OD2 | 2.15 | 0.46 |
| 20:QT:89:ARG:HH21 | 20:QT:104:LEU:HD21 | 1.80 | 0.46 |
| 24:QY:30:G:C2 | 24:QY:31:A:C8 | 3.03 | 0.46 |
| 53:R7:12:ARG:NH2 | 53:R7:44:PRO:HB3 | 2.31 | 0.46 |
| 25:RA:1687:G:N2 | 25:RA:1702:G:O6 | 2.48 | 0.46 |
| 25:RA:2187:G:H2' | 25:RA:2188:C:C6 | 2.49 | 0.46 |
| 25:RA:2785:C:H2' | 25:RA:2786:U:C6 | 2.51 | 0.46 |
| 25:RA:442:G:H1' | 29:RF:48:THR:HG21 | 1.96 | 0.46 |
| 25:RA:822:U:H2' | 25:RA:823:G:C8 | 2.49 | 0.46 |
| 29:RF:133:ASN:H | 29:RF:162:LEU:HD13 | 1.80 | 0.46 |
| 29:RF:73:ALA:HB3 | 29:RF:75:HIS:CE1 | 2.50 | 0.46 |
| 30:RG:81:LYS:O | 30:RG:82:LEU:HB2 | 2.14 | 0.46 |
| 33:RN:39:ARG:HD3 | 33:RN:48:MET:HE1 | 1.97 | 0.46 |
| 35:RP:94:GLU:O | 35:RP:96:THR:HG23 | 2.15 | 0.46 |
| 1:XA:22:G:H2' | 1:XA:23:C:C6 | 2.50 | 0.46 |
| 1:XA:411:A:H62 | 1:XA:413:G:H21 | 1.62 | 0.46 |
| 1:XA:768:A:H4' | 1:XA:1523:G:H21 | 1.80 | 0.46 |
| 4:XD:57:ARG:HB3 | 4:XD:206:PHE:CD1 | 2.51 | 0.46 |
| 9:XI:32:ASP:OD1 | 9:XI:33:PHE:N | 2.48 | 0.46 |
| 25:YA:1265:A:H8 | 25:YA:1265:A:OP1 | 1.98 | 0.46 |
| 25:YA:2033:A:O2' | 25:YA:2035:G:OP2 | 2.28 | 0.46 |
| 25:YA:2745:C:OP1 | 55:Y9:22:ARG:HB2 | 2.15 | 0.46 |
| 25:YA:2823:A:OP1 | 28:YE:113:PHE:HB2 | 2.14 | 0.46 |
| 25:YA:26:G:H1' | 25:YA:515:A:H61 | 1.80 | 0.46 |
| 25:YA:598:G:H5' | 35:YP:11:GLY:HA3 | 1.97 | 0.46 |
| 26:YB:95:U:H2' | 26:YB:96:G:H8 | 1.81 | 0.46 |
| 36:YQ:67:ARG:HD2 | 36:YQ:105:GLU:OE1 | 2.15 | 0.46 |
| 41:YV:22:VAL:HG12 | 41:YV:23:GLU:N | 2.30 | 0.46 |
| 45:YZ:5:LEU:HD11 | 45:YZ:44:PHE:HA | 1.98 | 0.46 |
| 1:QA:1009:G:C2 | 1:QA:1010:G:C8 | 3.03 | 0.46 |
| 1:QA:1111:A:H2' | 1:QA:1112:C:C6 | 2.50 | 0.46 |
| 1:QA:1175:G:H2' | 1:QA:1176:A:C8 | 2.50 | 0.46 |
| 1:QA:1305:G:N2 | 1:QA:1332:A:OP2 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1502:A:H2 | 1:QA:1505:G:H1 | 1.63 | 0.46 |
| 5:QE:115:VAL:HG11 | 5:QE:118:ILE:HB | 1.97 | 0.46 |
| 8:QH:102:ARG:NH1 | 8:QH:105:ARG:HH12 | 2.13 | 0.46 |
| 13:QM:12:ASN:O | 13:QM:13:LYS:HB2 | 2.14 | 0.46 |
| 25:RA:1769:G:O2' | 25:RA:1958:C:OP1 | 2.30 | 0.46 |
| 25:RA:2648:C:H2' | 25:RA:2649:U:H6 | 1.80 | 0.46 |
| 25:RA:2627:G:N2 | 25:RA:2777:G:OP1 | 2.43 | 0.46 |
| 25:RA:84:A:C2 | 25:RA:103:A:C5 | 3.04 | 0.46 |
| 25:RA:729:G:P | 27:RD:13:ARG:HD3 | 2.55 | 0.46 |
| 27:RD:35:LYS:HB3 | 27:RD:36:PRO:CD | 2.24 | 0.46 |
| 28:RE:50:GLY:HA2 | 28:RE:77:ILE:HA | 1.97 | 0.46 |
| 45:RZ:151:HIS:CB | 45:RZ:170:THR:HA | 2.46 | 0.46 |
| 1:XA:1372:U:H2' | 1:XA:1373:G:O4' | 2.15 | 0.46 |
| 1:XA:337:C:H2' | 1:XA:338:A:H8 | 1.80 | 0.46 |
| 1:XA:399:G:H2' | 1:XA:400:C:C6 | 2.51 | 0.46 |
| 1:XA:678:U:H2' | 1:XA:679:C:C6 | 2.49 | 0.46 |
| 1:XA:953:G:H5'' | 1:XA:965:A:H61 | 1.81 | 0.46 |
| 3:XC:150:LYS:HG3 | 3:XC:169:ALA:HB2 | 1.97 | 0.46 |
| 6:XF:30:LEU:HD23 | 6:XF:75:LEU:HD21 | 1.98 | 0.46 |
| 8:XH:51:VAL:HG11 | 8:XH:60:ARG:HH11 | 1.79 | 0.46 |
| 22:XW:52:C:H2' | 22:XW:53:G:C8 | 2.50 | 0.46 |
| 25:YA:1394:U:H4' | 25:YA:1603:A:H4' | 1.96 | 0.46 |
| 25:YA:2789:C:H1' | 25:YA:2892:A:H2 | 1.80 | 0.46 |
| 25:YA:92:G:H2' | 25:YA:93:C:H6 | 1.81 | 0.46 |
| 1:QA:1004:A:P | 1:QA:1025:U:H3 | 2.37 | 0.46 |
| 1:QA:1201:A:HO2' | 1:QA:1202:G:P | 2.38 | 0.46 |
| 1:QA:281:G:OP2 | 1:QA:281:G:H8 | 1.99 | 0.46 |
| 1:QA:406:G:H2' | 1:QA:407:G:C8 | 2.50 | 0.46 |
| 1:QA:501:C:OP1 | 12:QL:117:ARG:NH2 | 2.47 | 0.46 |
| 1:QA:610:G:C4 | 1:QA:611:A:C8 | 3.03 | 0.46 |
| 13:QM:86:CYS:SG | 13:QM:87:TYR:N | 2.88 | 0.46 |
| 1:QA:186:C:H5' | 20:QT:78:ALA:HB1 | 1.98 | 0.46 |
| 25:RA:1278:A:H2' | 25:RA:1279:G:C8 | 2.50 | 0.46 |
| 25:RA:1339:G:H5'' | 43:RX:16:LYS:HD3 | 1.97 | 0.46 |
| 25:RA:177:G:H5' | 25:RA:178:G:C8 | 2.50 | 0.46 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:H8 | 1.98 | 0.46 |
| 25:RA:2849:U:H5 | 39:RT:93:ARG:HH12 | 1.63 | 0.46 |
| 25:RA:52:A:H2' | 25:RA:53:A:C8 | 2.49 | 0.46 |
| 25:RA:694:U:OP1 | 27:RD:59:LYS:NZ | 2.36 | 0.46 |
| 25:RA:839:U:H2' | 25:RA:840:C:C6 | 2.50 | 0.46 |
| 25:RA:974(A):C:H4' | 25:RA:975:G:O5' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:RD:206:LEU:HA | 27:RD:211:ARG:HD3 | 1.97 | 0.46 |
| 29:RF:73:ALA:HB3 | 29:RF:75:HIS:HE1 | 1.79 | 0.46 |
| 35:RP:144:GLU:O | 35:RP:144:GLU:HG2 | 2.16 | 0.46 |
| 37:RR:45:ARG:HA | 37:RR:95:THR:HG21 | 1.97 | 0.46 |
| 40:RU:91:ASP:C | 40:RU:93:LYS:H | 2.17 | 0.46 |
| 1:XA:1325:C:H4' | 21:XU:17:THR:HG21 | 1.97 | 0.46 |
| 1:XA:385:C:H2' | 1:XA:386:C:C6 | 2.50 | 0.46 |
| 1:XA:410:G:H4' | 1:XA:411:A:OP1 | 2.16 | 0.46 |
| 1:XA:789:U:H1' | 1:XA:792:A:C2 | 2.43 | 0.46 |
| 1:XA:89:U:HO2' | 1:XA:90:C:P | 2.37 | 0.46 |
| 1:XA:940:C:H2' | 1:XA:941:G:C8 | 2.51 | 0.46 |
| 3:XC:9:GLY:HA2 | 3:XC:12:LEU:HG | 1.97 | 0.46 |
| 3:XC:153:VAL:HG22 | 3:XC:198:VAL:HG22 | 1.98 | 0.46 |
| 18:XR:58:LEU:HD23 | 18:XR:62:GLU:HB3 | 1.96 | 0.46 |
| 22:XW:20:G:H3' | 22:XW:21:U:C5 | 2.50 | 0.46 |
| 53:Y7:26:GLY:O | 53:Y7:30:VAL:HG23 | 2.15 | 0.46 |
| 55:Y9:25:VAL:O | 55:Y9:33:LYS:HG3 | 2.15 | 0.46 |
| 25:YA:1843:C:H2' | 25:YA:1844:C:C6 | 2.50 | 0.46 |
| 25:YA:2752:C:H3' | 25:YA:2753:A:C8 | 2.50 | 0.46 |
| 25:YA:277:C:H3' | 25:YA:278:A:C5' | 2.46 | 0.46 |
| 25:YA:2837:G:H2' | 25:YA:2838:G:C8 | 2.50 | 0.46 |
| 25:YA:319:C:H2' | 25:YA:320:A:C8 | 2.50 | 0.46 |
| 25:YA:413:C:H2' | 25:YA:414:C:C6 | 2.50 | 0.46 |
| 25:YA:503:A:H4' | 25:YA:504:U:H5' | 1.97 | 0.46 |
| 25:YA:631:A:OP1 | 54:Y8:46:ARG:NH2 | 2.49 | 0.46 |
| 25:YA:81:G:H2' | 25:YA:82:G:O4' | 2.15 | 0.46 |
| 29:YF:197:ASP:C | 29:YF:199:TRP:H | 2.19 | 0.46 |
| 40:YU:90:VAL:HG12 | 40:YU:91:ASP:N | 2.30 | 0.46 |
| 1:QA:1002:G:H2' | 1:QA:1003:G:C8 | 2.51 | 0.46 |
| 1:QA:1351:U:O2 | 1:QA:1371:G:N2 | 2.44 | 0.46 |
| 1:QA:643:C:C2 | 1:QA:644:G:C8 | 3.04 | 0.46 |
| 1:QA:922:G:H4' | 5:QE:20:GLN:HA | 1.97 | 0.46 |
| 25:RA:1045:A:O2' | 25:RA:1046:A:OP2 | 2.25 | 0.46 |
| 25:RA:1316:U:H2' | 25:RA:1317:A:C8 | 2.49 | 0.46 |
| 25:RA:1433:U:H3 | 25:RA:1560:G:H1 | 1.64 | 0.46 |
| 25:RA:1453:A:N6 | 25:RA:2702:U:H1' | 2.31 | 0.46 |
| 25:RA:2379:G:H2' | 25:RA:2380:C:C6 | 2.50 | 0.46 |
| 25:RA:2749:A:OP1 | 31:RH:4:ILE:HG23 | 2.15 | 0.46 |
| 25:RA:38:A:N3 | 29:RF:48:THR:OG1 | 2.48 | 0.46 |
| 25:RA:863:A:H2' | 25:RA:864:G:H8 | 1.81 | 0.46 |
| 25:RA:968:G:H2' | 25:RA:969:U:H6 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:125:PHE:HE2 | 30:RG:170:ARG:HB2 | 1.81 | 0.46 |
| 32:RI:5:LEU:HD21 | 32:RI:12:LEU:HB3 | 1.97 | 0.46 |
| 32:RI:13:GLY:HA3 | 32:RI:17:GLN:HB3 | 1.96 | 0.46 |
| 34:RO:97:ARG:O | 34:RO:97:ARG:HD3 | 2.15 | 0.46 |
| 1:XA:1190:G:H5' | 3:XC:176:HIS:HE1 | 1.81 | 0.46 |
| 1:XA:1504:G:OP1 | 1:XA:1507:A:H4' | 2.15 | 0.46 |
| 1:XA:272:C:H2' | 1:XA:273:A:C8 | 2.51 | 0.46 |
| 1:XA:484:G:H4' | 1:XA:485:G:O5' | 2.15 | 0.46 |
| 1:XA:782:A:H62 | 1:XA:800:G:H21 | 1.64 | 0.46 |
| 1:XA:892:A:O2' | 1:XA:1415:G:H4' | 2.16 | 0.46 |
| 5:XE:115:VAL:HG11 | 5:XE:118:ILE:HB | 1.97 | 0.46 |
| 15:XO:39:LEU:HD11 | 15:XO:52:SER:HB3 | 1.98 | 0.46 |
| 15:XO:15:PHE:CE2 | 15:XO:85:LEU:HD21 | 2.50 | 0.46 |
| 1:XA:719:C:O2' | 18:XR:49:LYS:HB3 | 2.15 | 0.46 |
| 19:XS:50:ALA:HB1 | 19:XS:57:HIS:HB3 | 1.98 | 0.46 |
| 25:YA:1167:U:H2' | 25:YA:1168:G:H8 | 1.80 | 0.46 |
| 25:YA:1518:C:H2' | 25:YA:1519:G:H8 | 1.80 | 0.46 |
| 25:YA:1766:U:H2' | 25:YA:1767:C:H6 | 1.81 | 0.46 |
| 25:YA:2291:U:H3 | 25:YA:2341:G:H1 | 1.64 | 0.46 |
| 25:YA:2306:C:H2' | 25:YA:2307:G:N2 | 2.30 | 0.46 |
| 25:YA:466:A:N3 | 25:YA:683:C:H1' | 2.31 | 0.46 |
| 27:YD:143:HIS:ND1 | 27:YD:194:GLY:O | 2.38 | 0.46 |
| 37:YR:100:LEU:HD11 | 37:YR:113:LEU:HB2 | 1.98 | 0.46 |
| 37:YR:3:HIS:O | 37:YR:5:LYS:N | 2.49 | 0.46 |
| 1:QA:1225:A:H2' | 1:QA:1225:A:N3 | 2.31 | 0.46 |
| 1:QA:1226:C:N4 | 13:QM:104:ARG:HH11 | 2.13 | 0.46 |
| 1:QA:865:A:H2' | 1:QA:866:C:C6 | 2.51 | 0.46 |
| 1:QA:921:U:O2' | 5:QE:19:MET:O | 2.32 | 0.46 |
| 13:QM:108:ARG:NE | 13:QM:114:ARG:HD2 | 2.31 | 0.46 |
| 17:QQ:45:HIS:CD2 | 17:QQ:47:PRO:HG3 | 2.51 | 0.46 |
| 25:RA:1137:G:H2' | 25:RA:1138:G:H8 | 1.80 | 0.46 |
| 25:RA:1408:C:H2' | 25:RA:1409:C:C6 | 2.49 | 0.46 |
| 25:RA:1441:G:H2' | 25:RA:1442:G:H8 | 1.81 | 0.46 |
| 25:RA:2115:G:N1 | 25:RA:2164:C:OP2 | 2.49 | 0.46 |
| 25:RA:2844:G:H3' | 25:RA:2845:G:H8 | 1.81 | 0.46 |
| 25:RA:336:C:O2' | 44:RY:35:TYR:OH | 2.34 | 0.46 |
| 25:RA:579:G:C2 | 25:RA:1262:A:C5 | 3.04 | 0.46 |
| 29:RF:126:VAL:H | 29:RF:195:ASP:HA | 1.80 | 0.46 |
| 1:XA:1218:C:H2' | 1:XA:1219:U:C6 | 2.50 | 0.46 |
| 1:XA:57:G:N2 | 1:XA:388:G:C6 | 2.84 | 0.46 |
| 1:XA:427:U:OP1 | 4:XD:13:ARG:NH2 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1109:C:H2' | 25:YA:1110:G:O4' | 2.15 | 0.46 |
| 25:YA:1499:C:H2' | 25:YA:1500:G:H8 | 1.81 | 0.46 |
| 25:YA:2123:G:H2' | 25:YA:2124:G:C8 | 2.51 | 0.46 |
| 27:YD:201:HIS:O | 27:YD:204:ILE:HG12 | 2.16 | 0.46 |
| 1:QA:1401:G:O6 | 1:QA:1504:G:N2 | 2.48 | 0.46 |
| 1:QA:28:G:O2' | 1:QA:296:U:OP1 | 2.34 | 0.46 |
| 1:QA:552:U:H2' | 1:QA:553:A:H8 | 1.81 | 0.46 |
| 8:QH:106:GLY:O | 8:QH:122:ARG:NH2 | 2.48 | 0.46 |
| 25:RA:1303:G:H1' | 25:RA:1641:A:N1 | 2.31 | 0.46 |
| 25:RA:2038:G:H2' | 25:RA:2039:C:C6 | 2.51 | 0.46 |
| 25:RA:251:A:C5 | 25:RA:252:G:H1' | 2.50 | 0.46 |
| 25:RA:911:A:H2' | 36:RQ:9:TYR:CE2 | 2.46 | 0.46 |
| 25:RA:92:G:H2' | 25:RA:93:C:C6 | 2.50 | 0.46 |
| 30:RG:125:PHE:CE2 | 30:RG:170:ARG:HB2 | 2.51 | 0.46 |
| 35:RP:101:VAL:CB | 35:RP:106:LEU:HB2 | 2.43 | 0.46 |
| 38:RS:30:ARG:HD2 | 38:RS:97:ARG:HD3 | 1.97 | 0.46 |
| 40:RU:81:HIS:NE2 | 40:RU:85:LYS:HE3 | 2.30 | 0.46 |
| 1:XA:1229:A:OP2 | 13:XM:114:ARG:NH1 | 2.47 | 0.46 |
| 1:XA:1410:G:H2' | 1:XA:1411:C:C6 | 2.51 | 0.46 |
| 1:XA:323:U:OP1 | 20:XT:26:ASN:ND2 | 2.48 | 0.46 |
| 1:XA:777:A:H2' | 1:XA:778:G:H8 | 1.81 | 0.46 |
| 2:XB:101:MET:HA | 2:XB:108:ILE:HG13 | 1.97 | 0.46 |
| 8:XH:17:THR:HB | 8:XH:78:GLN:OE1 | 2.16 | 0.46 |
| 17:XQ:83:ASP:OD1 | 17:XQ:84:LEU:N | 2.49 | 0.46 |
| 18:XR:50:ILE:HG13 | 18:XR:74:ARG:HH22 | 1.80 | 0.46 |
| 31:YH:149:ARG:CZ | 55:Y9:20:HIS:H | 2.29 | 0.46 |
| 31:YH:149:ARG:NH2 | 55:Y9:20:HIS:H | 2.13 | 0.46 |
| 55:Y9:4:ARG:HG3 | 55:Y9:34:GLN:HG2 | 1.98 | 0.46 |
| 25:YA:2689:U:H5' | 25:YA:2713:A:H2 | 1.81 | 0.46 |
| 25:YA:363(F):A:H4' | 25:YA:364:C:H5' | 1.98 | 0.46 |
| 25:YA:381:G:C6 | 25:YA:394:A:N1 | 2.84 | 0.46 |
| 25:YA:521:G:H2' | 25:YA:522:G:C8 | 2.51 | 0.46 |
| 25:YA:587:C:N3 | 35:YP:33:ARG:NH2 | 2.62 | 0.46 |
| 25:YA:639:U:H2' | 25:YA:640:C:H6 | 1.81 | 0.46 |
| 26:YB:44:G:H1' | 26:YB:47:C:H41 | 1.80 | 0.46 |
| 28:YE:36:ARG:NH1 | 28:YE:85:ASN:OD1 | 2.49 | 0.46 |
| 30:YG:143:GLU:OE2 | 50:Y4:26:SER:OG | 2.23 | 0.46 |
| 36:YQ:30:GLY:HA2 | 36:YQ:107:ALA:HB2 | 1.97 | 0.46 |
| 39:YT:101:PHE:HD2 | 39:YT:105:LEU:HD21 | 1.80 | 0.46 |
| 1:QA:113:G:H2' | 1:QA:114:U:C6 | 2.51 | 0.46 |
| 1:QA:279:A:OP1 | 1:QA:280:C:O2' | 2.25 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:868:C:H2' | 1:QA:869:G:O4' | 2.15 | 0.46 |
| 8:QH:121:ASP:OD1 | 8:QH:122:ARG:N | 2.49 | 0.46 |
| 13:QM:4:ILE:HA | 13:QM:57:ARG:HG2 | 1.97 | 0.46 |
| 54:R8:29:LYS:HB2 | 54:R8:33:ASN:HD21 | 1.81 | 0.46 |
| 25:RA:327:G:H2' | 25:RA:328:U:C6 | 2.50 | 0.46 |
| 25:RA:2313:C:H5'' | 30:RG:91:ARG:HD3 | 1.97 | 0.46 |
| 41:RV:64:HIS:ND1 | 41:RV:92:THR:HG22 | 2.31 | 0.46 |
| 43:RX:11:PRO:HD3 | 48:R2:37:PHE:CD1 | 2.50 | 0.46 |
| 1:XA:1221:G:O3' | 19:XS:77:THR:HG21 | 2.16 | 0.46 |
| 1:XA:1293:G:H2' | 1:XA:1294:G:C8 | 2.51 | 0.46 |
| 1:XA:650:G:H2' | 1:XA:651:C:C6 | 2.50 | 0.46 |
| 1:XA:74:C:H2' | 1:XA:75:C:C6 | 2.50 | 0.46 |
| 1:XA:619:U:N3 | 4:XD:134:ASP:OD1 | 2.44 | 0.46 |
| 5:XE:87:SER:HB3 | 5:XE:131:ILE:HD13 | 1.97 | 0.46 |
| 11:XK:87:THR:HA | 11:XK:91:ARG:HD2 | 1.98 | 0.46 |
| 30:YG:3:LEU:HD11 | 50:Y4:25:TYR:HE2 | 1.81 | 0.46 |
| 25:YA:2093:G:H2' | 25:YA:2094:G:C8 | 2.51 | 0.46 |
| 25:YA:2099:U:H2' | 25:YA:2100:G:H8 | 1.80 | 0.46 |
| 25:YA:2471:C:H3' | 25:YA:2472:G:H8 | 1.80 | 0.46 |
| 25:YA:296:C:H2' | 25:YA:297:C:C6 | 2.51 | 0.46 |
| 25:YA:639:U:H2' | 25:YA:640:C:C6 | 2.51 | 0.46 |
| 29:YF:148:LEU:HD22 | 29:YF:154:VAL:HG21 | 1.98 | 0.46 |
| 30:YG:40:ASN:HD22 | 30:YG:41:GLN:H | 1.64 | 0.46 |
| 33:YN:96:GLU:HB2 | 33:YN:122:VAL:HG12 | 1.97 | 0.46 |
| 36:YQ:30:GLY:CA | 36:YQ:107:ALA:HB2 | 2.45 | 0.46 |
| 36:YQ:4:PRO:HG3 | 36:YQ:69:PHE:HE2 | 1.80 | 0.46 |
| 34:YO:76:ALA:HB3 | 39:YT:75:ILE:HD12 | 1.96 | 0.46 |
| 1:QA:1512:U:H2' | 1:QA:1513:A:H8 | 1.81 | 0.46 |
| 6:QF:12:PRO:HG3 | 6:QF:57:GLN:HG3 | 1.98 | 0.46 |
| 6:QF:97:PHE:CD2 | 18:QR:31:LEU:HD21 | 2.51 | 0.46 |
| 22:QW:49:C:N3 | 22:QW:60:A:H1' | 2.30 | 0.46 |
| 25:RA:1448:G:H5' | 25:RA:1449:A:OP1 | 2.15 | 0.46 |
| 25:RA:1449:A:C4 | 25:RA:1529:A:H2 | 2.34 | 0.46 |
| 25:RA:1539:G:H2' | 25:RA:1540:G:C8 | 2.51 | 0.46 |
| 25:RA:1689:A:H62 | 25:RA:1698:A:H2 | 1.64 | 0.46 |
| 25:RA:1791:A:H3' | 25:RA:1792:G:H8 | 1.81 | 0.46 |
| 25:RA:2532:G:H2' | 25:RA:2533:A:C8 | 2.51 | 0.46 |
| 25:RA:2556:C:H2' | 25:RA:2557:G:O4' | 2.16 | 0.46 |
| 25:RA:815:C:OP2 | 41:RV:83:ARG:NH1 | 2.49 | 0.46 |
| 30:RG:15:VAL:HG21 | 30:RG:176:LEU:HD23 | 1.98 | 0.46 |
| 1:XA:1307:U:O4 | 1:XA:1331:G:N2 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:78:G:C6 | 1:XA:92:G:C6 | 3.04 | 0.46 |
| 1:XA:939:G:H2' | 1:XA:940:C:C6 | 2.51 | 0.46 |
| 4:XD:155:LEU:O | 4:XD:158:ILE:N | 2.48 | 0.46 |
| 10:XJ:51:ARG:HG3 | 10:XJ:60:ARG:HA | 1.97 | 0.46 |
| 13:XM:87:TYR:O | 13:XM:90:LEU:HG | 2.16 | 0.46 |
| 15:XO:26:GLU:HG3 | 15:XO:81:LEU:HD22 | 1.98 | 0.46 |
| 25:YA:2526:G:H4' | 55:Y9:27:CYS:SG | 2.56 | 0.46 |
| 25:YA:1026:U:H1' | 25:YA:1027:A:O5' | 2.16 | 0.46 |
| 25:YA:1042:G:H2' | 25:YA:1043:C:C6 | 2.51 | 0.46 |
| 25:YA:1113:U:H2' | 25:YA:1114:G:C8 | 2.51 | 0.46 |
| 25:YA:1541:U:H2' | 25:YA:1542:G:O4' | 2.15 | 0.46 |
| 25:YA:1831:G:H2' | 25:YA:1832:C:C6 | 2.51 | 0.46 |
| 25:YA:2563:U:H1' | 25:YA:2566:A:N6 | 2.31 | 0.46 |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:C8 | 2.51 | 0.46 |
| 25:YA:583:G:OP2 | 40:YU:10:ARG:HD2 | 2.16 | 0.46 |
| 25:YA:907:U:O2' | 36:YQ:101:ARG:NH2 | 2.49 | 0.46 |
| 29:YF:9:ILE:HG12 | 29:YF:123:LEU:HD23 | 1.97 | 0.46 |
| 25:YA:1138:G:H21 | 33:YN:106:MET:HE3 | 1.81 | 0.46 |
| 36:YQ:4:PRO:HG3 | 36:YQ:69:PHE:CE2 | 2.51 | 0.46 |
| 1:QA:728:A:H2' | 1:QA:729:A:H8 | 1.81 | 0.46 |
| 4:QD:10:ARG:HG3 | 4:QD:40:PRO:HG3 | 1.98 | 0.46 |
| 7:QG:66:VAL:HG12 | 7:QG:70:LYS:HE3 | 1.98 | 0.46 |
| 22:QW:52:C:H2' | 22:QW:53:G:C8 | 2.51 | 0.46 |
| 55:R9:2:LYS:HD3 | 55:R9:32:HIS:HA | 1.98 | 0.46 |
| 25:RA:1210:A:H4' | 25:RA:1211:U:O5' | 2.16 | 0.46 |
| 25:RA:1268:A:H2' | 25:RA:1269:A:O4' | 2.15 | 0.46 |
| 25:RA:1281:G:H2' | 25:RA:1282:U:C6 | 2.50 | 0.46 |
| 25:RA:127:A:H5'' | 25:RA:128:C:C6 | 2.51 | 0.46 |
| 25:RA:2150:U:H2' | 25:RA:2151:G:H8 | 1.81 | 0.46 |
| 25:RA:492:A:H2' | 25:RA:493:G:O4' | 2.15 | 0.46 |
| 34:RO:22:ILE:HG12 | 34:RO:41:ALA:HA | 1.98 | 0.46 |
| 25:RA:910:A:C5 | 36:RQ:13:GLN:HG3 | 2.50 | 0.46 |
| 43:RX:26:TYR:CD2 | 43:RX:89:ILE:HD12 | 2.48 | 0.46 |
| 1:XA:1107:C:C4 | 1:XA:1108:G:C8 | 3.04 | 0.46 |
| 1:XA:769:G:H4' | 1:XA:1513:A:H4' | 1.98 | 0.46 |
| 6:XF:47:ARG:NH2 | 6:XF:57:GLN:OE1 | 2.49 | 0.46 |
| 7:XG:152:ALA:O | 7:XG:155:ARG:HG3 | 2.16 | 0.46 |
| 9:XI:42:ARG:HH22 | 9:XI:75:ASP:CG | 2.19 | 0.46 |
| 22:XW:2:G:H2' | 22:XW:3:C:C6 | 2.51 | 0.46 |
| 25:YA:1196:C:C2 | 25:YA:1197:G:C8 | 3.04 | 0.46 |
| 25:YA:1231:G:H2' | 25:YA:1232:G:H8 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:2028:U:H2' | 25:YA:2029:G:C8 | 2.51 | 0.46 |
| 25:YA:2050:C:H2' | 25:YA:2051:A:C8 | 2.51 | 0.46 |
| 25:YA:623:G:H2' | 25:YA:624:C:C6 | 2.51 | 0.46 |
| 25:YA:968:G:H2' | 25:YA:969:U:H6 | 1.81 | 0.46 |
| 27:YD:206:LEU:HA | 27:YD:211:ARG:HD3 | 1.97 | 0.46 |
| 25:YA:773:U:H4' | 27:YD:47:GLY:HA2 | 1.97 | 0.46 |
| 38:YS:110:LEU:HB3 | 38:YS:112:PHE:CE1 | 2.51 | 0.46 |
| 39:YT:26:ASP:O | 39:YT:49:VAL:HG12 | 2.16 | 0.46 |
| 42:YW:110:LYS:HG3 | 42:YW:111:HIS:ND1 | 2.31 | 0.46 |
| 1:QA:1004:A:N1 | 1:QA:1025:U:H1' | 2.31 | 0.45 |
| 1:QA:1391:U:H2' | 1:QA:1392:G:C8 | 2.51 | 0.45 |
| 1:QA:580:U:H2' | 1:QA:581:G:O4' | 2.16 | 0.45 |
| 1:QA:645:C:H2' | 1:QA:646:U:H6 | 1.81 | 0.45 |
| 2:QB:30:ARG:HH21 | 2:QB:194:PRO:HG2 | 1.81 | 0.45 |
| 4:QD:167:GLY:HA2 | 27:YD:135:PHE:CZ | 2.51 | 0.45 |
| 10:QJ:51:ARG:NH2 | 10:QJ:61:GLU:HB3 | 2.31 | 0.45 |
| 12:QL:33:ARG:NH2 | 12:QL:61:THR:OG1 | 2.49 | 0.45 |
| 25:RA:1541:U:H2' | 25:RA:1542:G:O4' | 2.16 | 0.45 |
| 25:RA:1704:G:H2' | 25:RA:1705:G:H8 | 1.81 | 0.45 |
| 25:RA:2235:G:H2' | 25:RA:2236:C:C6 | 2.51 | 0.45 |
| 25:RA:2795:G:H3' | 25:RA:2797:U:C5' | 2.46 | 0.45 |
| 25:RA:678:C:H2' | 25:RA:679:C:H6 | 1.81 | 0.45 |
| 25:RA:834:C:C2 | 25:RA:835:A:C8 | 3.04 | 0.45 |
| 25:RA:851:U:H2' | 25:RA:852:G:H8 | 1.81 | 0.45 |
| 25:RA:94:G:H21 | 48:R2:47:ASN:HD22 | 1.64 | 0.45 |
| 26:RB:42:C:O2 | 30:RG:93:THR:N | 2.42 | 0.45 |
| 44:RY:83:THR:HG21 | 44:RY:99:CYS:SG | 2.56 | 0.45 |
| 45:RZ:45:ASP:OD1 | 45:RZ:49:ARG:NE | 2.49 | 0.45 |
| 1:XA:1120:G:H2' | 1:XA:1121:U:C6 | 2.52 | 0.45 |
| 1:XA:1315:U:H2' | 1:XA:1316:G:O4' | 2.17 | 0.45 |
| 1:XA:165:C:H2' | 1:XA:166:G:H8 | 1.80 | 0.45 |
| 55:Y9:26:ILE:CG2 | 55:Y9:33:LYS:HE3 | 2.45 | 0.45 |
| 25:YA:1028:A:H2' | 25:YA:1029:A:C8 | 2.50 | 0.45 |
| 25:YA:1065:U:O2 | 25:YA:1074:G:N1 | 2.49 | 0.45 |
| 25:YA:118:A:N3 | 25:YA:178:G:H1' | 2.31 | 0.45 |
| 25:YA:1939:U:OP1 | 25:YA:2604:U:O2' | 2.23 | 0.45 |
| 25:YA:2119:A:H61 | 25:YA:2168:G:N2 | 2.14 | 0.45 |
| 25:YA:2446:G:N2 | 25:YA:2449:U:O2 | 2.48 | 0.45 |
| 25:YA:742:G:H2' | 25:YA:743:G:H8 | 1.81 | 0.45 |
| 25:YA:870:A:H2' | 25:YA:871:U:O4' | 2.16 | 0.45 |
| 27:YD:32:SER:HA | 27:YD:35:LYS:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:YS:89:ARG:HD2 | 38:YS:94:TYR:HB2 | 1.96 | 0.45 |
| 41:YV:77:ALA:O | 41:YV:79:VAL:HG23 | 2.16 | 0.45 |
| 1:QA:1229:A:H2' | 1:QA:1230:C:C6 | 2.51 | 0.45 |
| 1:QA:1372:U:H5'' | 9:QI:71:SER:HB3 | 1.98 | 0.45 |
| 1:QA:639:G:H2' | 1:QA:640:A:H8 | 1.82 | 0.45 |
| 1:QA:726:C:H2' | 1:QA:727:G:H8 | 1.80 | 0.45 |
| 2:QB:163:PHE:HD1 | 2:QB:185:ILE:HG13 | 1.82 | 0.45 |
| 11:QK:27:ASN:OD1 | 11:QK:28:THR:N | 2.48 | 0.45 |
| 22:QV:36:A:H2' | 22:QV:37:U:C6 | 2.52 | 0.45 |
| 49:R3:16:PRO:HB2 | 49:R3:18:ASP:OD1 | 2.17 | 0.45 |
| 25:RA:1149:G:H2' | 25:RA:1150:C:C6 | 2.51 | 0.45 |
| 25:RA:1164:G:H2' | 25:RA:1165:U:H6 | 1.79 | 0.45 |
| 25:RA:147:U:H2' | 25:RA:148:C:C6 | 2.52 | 0.45 |
| 25:RA:743:G:O2' | 25:RA:1659:U:OP1 | 2.32 | 0.45 |
| 25:RA:2119:A:N6 | 25:RA:2170:A:N7 | 2.62 | 0.45 |
| 26:RB:8:U:H3 | 26:RB:112:G:H1 | 1.65 | 0.45 |
| 31:RH:8:PRO:HG2 | 31:RH:69:ARG:HH21 | 1.82 | 0.45 |
| 38:RS:14:VAL:HG11 | 38:RS:90:GLY:O | 2.16 | 0.45 |
| 1:XA:132:C:H4' | 1:XA:262:A:H1' | 1.97 | 0.45 |
| 1:XA:64:G:H5'' | 1:XA:65:U:OP1 | 2.16 | 0.45 |
| 1:XA:678:U:H2' | 1:XA:679:C:H6 | 1.81 | 0.45 |
| 1:XA:97:U:H2' | 1:XA:99:C:C6 | 2.52 | 0.45 |
| 3:XC:5:ILE:HD11 | 14:XN:49:HIS:HE1 | 1.80 | 0.45 |
| 22:XV:29:C:H2' | 22:XV:30:G:H8 | 1.81 | 0.45 |
| 48:Y2:10:LEU:HD21 | 48:Y2:59:ARG:HD2 | 1.98 | 0.45 |
| 31:YH:149:ARG:HH21 | 55:Y9:20:HIS:H | 1.63 | 0.45 |
| 25:YA:1771:C:H2' | 25:YA:1772:G:C8 | 2.51 | 0.45 |
| 25:YA:2062:A:N3 | 25:YA:2062:A:H2' | 2.29 | 0.45 |
| 25:YA:2567:G:H2' | 25:YA:2568:C:C6 | 2.51 | 0.45 |
| 25:YA:27:G:HO2' | 25:YA:28:A:H8 | 1.64 | 0.45 |
| 25:YA:288:C:H2' | 25:YA:289:A:C8 | 2.45 | 0.45 |
| 30:YG:71:THR:N | 30:YG:89:GLY:O | 2.49 | 0.45 |
| 1:QA:166:G:H2' | 1:QA:167:G:H8 | 1.81 | 0.45 |
| 1:QA:422:C:HO2' | 1:QA:423:G:N2 | 2.15 | 0.45 |
| 3:QC:20:SER:OG | 3:QC:22:TRP:NE1 | 2.48 | 0.45 |
| 7:QG:15:ASP:OD1 | 7:QG:16:LEU:N | 2.49 | 0.45 |
| 13:QM:16:ASP:OD1 | 13:QM:17:VAL:N | 2.49 | 0.45 |
| 46:R0:48:GLY:HA3 | 46:R0:80:HIS:CE1 | 2.51 | 0.45 |
| 25:RA:1257:C:H2' | 25:RA:1258:C:C6 | 2.51 | 0.45 |
| 25:RA:2563:U:H1' | 25:RA:2566:A:N6 | 2.31 | 0.45 |
| 25:RA:639:U:H2' | 25:RA:640:C:H6 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:RD:25:THR:HG22 | 27:RD:82:ILE:H | 1.82 | 0.45 |
| 28:RE:38:THR:OG1 | 28:RE:40:GLU:OE1 | 2.34 | 0.45 |
| 28:RE:48:GLN:OE1 | 28:RE:64:LYS:NZ | 2.46 | 0.45 |
| 32:RI:115:ALA:HB2 | 32:RI:131:LYS:HE2 | 1.98 | 0.45 |
| 32:RI:144:VAL:HG22 | 32:RI:145:VAL:H | 1.80 | 0.45 |
| 39:RT:120:ARG:HA | 39:RT:123:GLN:HB2 | 1.98 | 0.45 |
| 39:RT:65:LYS:O | 39:RT:72:VAL:N | 2.43 | 0.45 |
| 1:XA:1004:A:HO2' | 1:XA:1036:G:H1 | 1.64 | 0.45 |
| 1:XA:1435:G:H2' | 1:XA:1436:U:H6 | 1.81 | 0.45 |
| 1:XA:363:A:N1 | 12:XL:31:PRO:HD2 | 2.31 | 0.45 |
| 1:XA:981:U:H2' | 1:XA:982:U:C5 | 2.52 | 0.45 |
| 10:XJ:39:PRO:HA | 10:XJ:70:ARG:HD3 | 1.98 | 0.45 |
| 11:XK:43:SER:HB3 | 11:XK:68:ALA:HB2 | 1.98 | 0.45 |
| 1:XA:468:A:H5'' | 16:XP:80:PHE:HB3 | 1.99 | 0.45 |
| 21:XU:6:ARG:HE | 21:XU:15:ARG:NH2 | 2.13 | 0.45 |
| 46:Y0:23:VAL:HB | 46:Y0:26:TYR:HE1 | 1.80 | 0.45 |
| 49:Y3:15:TYR:CE2 | 49:Y3:53:LEU:HD21 | 2.51 | 0.45 |
| 25:YA:1308:A:H3' | 25:YA:1309:G:H8 | 1.80 | 0.45 |
| 25:YA:1365:A:O2' | 47:Y1:11:ARG:NH2 | 2.39 | 0.45 |
| 25:YA:1694:C:H4' | 25:YA:1695:G:O5' | 2.15 | 0.45 |
| 25:YA:1790:C:H5'' | 25:YA:1791:A:OP1 | 2.16 | 0.45 |
| 25:YA:2074:U:H2' | 25:YA:2075:U:H6 | 1.82 | 0.45 |
| 25:YA:2292:C:H2' | 25:YA:2293:C:H6 | 1.80 | 0.45 |
| 25:YA:2392:A:H2 | 25:YA:2424:C:H42 | 1.64 | 0.45 |
| 27:YD:9:TYR:HD2 | 27:YD:10:THR:HG23 | 1.81 | 0.45 |
| 34:YO:97:ARG:O | 34:YO:97:ARG:HD3 | 2.16 | 0.45 |
| 28:YE:14:ILE:HG13 | 39:YT:14:TYR:HE2 | 1.82 | 0.45 |
| 25:YA:1216:G:OP1 | 40:YU:8:VAL:HG23 | 2.16 | 0.45 |
| 42:YW:111:HIS:CD2 | 42:YW:113:LYS:H | 2.34 | 0.45 |
| 1:QA:1004:A:H1' | 1:QA:1036:G:H22 | 1.80 | 0.45 |
| 1:QA:114:U:H2' | 1:QA:115:G:C8 | 2.52 | 0.45 |
| 1:QA:139:G:H2' | 1:QA:140:A:C8 | 2.51 | 0.45 |
| 1:QA:410:G:H4' | 1:QA:411:A:OP1 | 2.16 | 0.45 |
| 1:QA:541:G:H2' | 1:QA:542:G:H8 | 1.82 | 0.45 |
| 2:QB:74:LYS:O | 2:QB:78:GLN:HG3 | 2.17 | 0.45 |
| 15:QO:78:TYR:CZ | 15:QO:82:ILE:HD11 | 2.51 | 0.45 |
| 18:QR:51:LEU:HD22 | 18:QR:55:ARG:HD2 | 1.98 | 0.45 |
| 25:RA:1031:G:N2 | 55:R9:20:HIS:ND1 | 2.64 | 0.45 |
| 25:RA:17:G:H4' | 40:RU:25:TRP:NE1 | 2.27 | 0.45 |
| 25:RA:26:G:H1' | 25:RA:515:A:H61 | 1.80 | 0.45 |
| 25:RA:2841:C:H2' | 25:RA:2842:G:H8 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:519:U:H2' | 25:RA:520:G:H8 | 1.81 | 0.45 |
| 27:RD:108:PRO:HD2 | 27:RD:111:LEU:HD22 | 1.98 | 0.45 |
| 25:RA:2680:C:O2' | 28:RE:11:MET:SD | 2.74 | 0.45 |
| 28:RE:131:ALA:O | 28:RE:134:ILE:HG13 | 2.16 | 0.45 |
| 28:RE:36:ARG:NH1 | 28:RE:85:ASN:OD1 | 2.50 | 0.45 |
| 41:RV:22:VAL:HG12 | 41:RV:23:GLU:N | 2.30 | 0.45 |
| 1:XA:1213:A:N1 | 1:XA:1215:G:H1' | 2.31 | 0.45 |
| 1:XA:1399:C:C2 | 1:XA:1502:A:N6 | 2.85 | 0.45 |
| 1:XA:389:A:H3' | 1:XA:390:C:H6 | 1.81 | 0.45 |
| 46:Y0:46:LYS:HB2 | 46:Y0:78:TYR:CD1 | 2.52 | 0.45 |
| 25:YA:1062:G:C8 | 25:YA:1088:A:C4 | 3.04 | 0.45 |
| 25:YA:1423:G:H2' | 25:YA:1424:G:H8 | 1.82 | 0.45 |
| 25:YA:1853:A:N6 | 25:YA:1889:A:N7 | 2.64 | 0.45 |
| 25:YA:195:A:H5'' | 25:YA:196:A:O5' | 2.16 | 0.45 |
| 25:YA:2040:C:H2' | 25:YA:2041:U:C6 | 2.51 | 0.45 |
| 25:YA:2131:G:H1' | 25:YA:2158:A:N6 | 2.31 | 0.45 |
| 25:YA:2528:U:O3' | 25:YA:2529:G:H8 | 2.00 | 0.45 |
| 25:YA:465:G:N2 | 25:YA:684:G:H1' | 2.31 | 0.45 |
| 25:YA:528:A:C2 | 25:YA:2042:A:H2' | 2.51 | 0.45 |
| 29:YF:155:LEU:HD12 | 29:YF:174:VAL:O | 2.17 | 0.45 |
| 29:YF:78:ILE:HA | 29:YF:83:PHE:HD2 | 1.80 | 0.45 |
| 1:QA:1060:C:H5'' | 10:QJ:51:ARG:HG2 | 1.98 | 0.45 |
| 1:QA:1336:C:H1' | 1:QA:1337:G:C2 | 2.51 | 0.45 |
| 1:QA:513:C:H2' | 1:QA:514:C:C6 | 2.51 | 0.45 |
| 13:QM:84:ILE:HD13 | 19:QS:65:ASN:HD21 | 1.81 | 0.45 |
| 55:R9:13:LYS:HD2 | 55:R9:28:GLU:OE2 | 2.15 | 0.45 |
| 25:RA:1771:C:H2' | 25:RA:1772:G:C8 | 2.50 | 0.45 |
| 25:RA:2461:C:C2 | 25:RA:2462:U:C5 | 3.05 | 0.45 |
| 25:RA:687:C:H2' | 25:RA:688:U:O4' | 2.15 | 0.45 |
| 30:RG:60:LEU:HD22 | 30:RG:68:PRO:HB3 | 1.98 | 0.45 |
| 1:XA:1241:G:H2' | 1:XA:1242:C:C6 | 2.51 | 0.45 |
| 1:XA:481:G:HO2' | 1:XA:482:A:P | 2.40 | 0.45 |
| 1:XA:501:C:H2' | 1:XA:502:G:C8 | 2.51 | 0.45 |
| 21:XU:10:ARG:HA | 21:XU:13:ILE:HD12 | 1.98 | 0.45 |
| 25:YA:2756:U:O5' | 55:Y9:3:VAL:HG21 | 2.16 | 0.45 |
| 25:YA:1000:A:OP2 | 25:YA:1154:G:N1 | 2.42 | 0.45 |
| 25:YA:1069:A:H2' | 25:YA:1073:A:N7 | 2.31 | 0.45 |
| 25:YA:749:C:H5' | 25:YA:1271:G:H1' | 1.98 | 0.45 |
| 25:YA:1588:C:H2' | 25:YA:1589:C:H6 | 1.82 | 0.45 |
| 25:YA:1727:U:H2' | 25:YA:1728:G:O4' | 2.17 | 0.45 |
| 25:YA:2803:C:H2' | 25:YA:2804:C:C6 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:YA:34:C:H5' | 25:YA:35:G:OP2 | 2.17 | 0.45 |
| 29:YF:89:VAL:HG12 | 29:YF:90:PHE:CD2 | 2.51 | 0.45 |
| 32:YI:27:ARG:HB2 | 47:Y1:71:TYR:CE2 | 2.51 | 0.45 |
| 25:YA:483:A:O2' | 44:YY:49:VAL:O | 2.22 | 0.45 |
| 1:QA:1270:C:H2' | 1:QA:1271:G:H8 | 1.82 | 0.45 |
| 2:QB:207:ALA:O | 2:QB:209:ARG:N | 2.49 | 0.45 |
| 12:QL:66:VAL:HG21 | 12:QL:98:TYR:CE2 | 2.51 | 0.45 |
| 13:QM:88:ARG:HD3 | 19:QS:69:HIS:HE1 | 1.81 | 0.45 |
| 13:QM:87:TYR:O | 13:QM:90:LEU:HG | 2.17 | 0.45 |
| 20:QT:20:LEU:O | 20:QT:23:ARG:HG2 | 2.17 | 0.45 |
| 49:R3:40:THR:HB | 49:R3:43:ILE:HG12 | 1.98 | 0.45 |
| 25:RA:1444(A):A:H4' | 25:RA:1460:A:O2' | 2.16 | 0.45 |
| 25:RA:1535:U:H2' | 25:RA:1536:A:C8 | 2.52 | 0.45 |
| 25:RA:2561:A:H5'' | 34:RO:57:VAL:HG11 | 1.99 | 0.45 |
| 25:RA:288:C:H2' | 25:RA:289:A:C8 | 2.51 | 0.45 |
| 25:RA:813:U:C5 | 35:RP:25:SER:HB3 | 2.52 | 0.45 |
| 25:RA:940:G:H2' | 25:RA:941:A:O4' | 2.17 | 0.45 |
| 25:RA:1327:C:O2' | 37:RR:105:ARG:NH1 | 2.46 | 0.45 |
| 1:XA:1206:G:C4 | 1:XA:1207:G:C8 | 3.05 | 0.45 |
| 1:XA:287:U:H2' | 1:XA:288:A:H8 | 1.81 | 0.45 |
| 1:XA:413:G:OP2 | 1:XA:413:G:H8 | 1.99 | 0.45 |
| 1:XA:554:C:H2' | 1:XA:555:C:H6 | 1.82 | 0.45 |
| 2:XB:134:GLU:HA | 2:XB:137:ARG:HG2 | 1.98 | 0.45 |
| 6:XF:21:LEU:O | 6:XF:25:ILE:HG12 | 2.16 | 0.45 |
| 25:YA:2755:C:C5' | 55:Y9:3:VAL:HG13 | 2.46 | 0.45 |
| 25:YA:1142(A):A:C4 | 25:YA:1144:G:C8 | 3.04 | 0.45 |
| 25:YA:1681:G:HO2' | 25:YA:1762:A:HO2' | 1.61 | 0.45 |
| 25:YA:1869:G:N1 | 25:YA:1872:A:OP2 | 2.39 | 0.45 |
| 25:YA:2011:U:OP2 | 42:YW:16:LYS:NZ | 2.36 | 0.45 |
| 25:YA:620:G:H4' | 25:YA:621:A:H5'' | 1.98 | 0.45 |
| 28:YE:45:THR:O | 28:YE:83:ASP:N | 2.49 | 0.45 |
| 29:YF:116:ASP:OD1 | 29:YF:119:ARG:NH2 | 2.48 | 0.45 |
| 36:YQ:58:PHE:HD2 | 36:YQ:61:GLY:HA3 | 1.81 | 0.45 |
| 25:YA:1262:A:OP2 | 42:YW:97:LYS:NZ | 2.48 | 0.45 |
| 45:YZ:145:GLU:HG3 | 45:YZ:146:ILE:HG12 | 1.98 | 0.45 |
| 1:QA:939:G:H2' | 1:QA:940:C:C6 | 2.51 | 0.45 |
| 2:QB:97:TRP:HZ3 | 2:QB:172:ILE:HG22 | 1.82 | 0.45 |
| 4:QD:190:ASP:OD1 | 4:QD:191:ARG:N | 2.44 | 0.45 |
| 25:RA:1131:G:OP1 | 33:RN:80:GLY:N | 2.42 | 0.45 |
| 25:RA:1438:U:H2' | 25:RA:1439:A:C8 | 2.50 | 0.45 |
| 25:RA:270(S):G:H2' | 25:RA:270(T):G:C8 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:271(B):G:H1' | 25:RA:271(C):U:OP2 | 2.17 | 0.45 |
| 25:RA:307:G:H21 | 25:RA:330:A:H62 | 1.65 | 0.45 |
| 25:RA:414:C:H2' | 25:RA:415:A:H8 | 1.82 | 0.45 |
| 25:RA:265:A:N6 | 25:RA:428:A:C8 | 2.84 | 0.45 |
| 25:RA:581:C:H2' | 25:RA:582:G:C8 | 2.51 | 0.45 |
| 25:RA:729:G:H5' | 25:RA:730:C:H5'' | 1.98 | 0.45 |
| 26:RB:109:G:H2' | 26:RB:110:G:C8 | 2.51 | 0.45 |
| 28:RE:116:VAL:HG23 | 28:RE:157:ALA:HB2 | 1.98 | 0.45 |
| 1:XA:595:G:H21 | 1:XA:596:C:N4 | 2.15 | 0.45 |
| 15:XO:36:ILE:HG23 | 15:XO:56:LEU:HD11 | 1.98 | 0.45 |
| 47:Y1:89:GLU:O | 47:Y1:93:GLU:HB2 | 2.17 | 0.45 |
| 25:YA:1264:G:H3' | 25:YA:1265:A:H5'' | 1.99 | 0.45 |
| 25:YA:177:G:H3' | 25:YA:178:G:H8 | 1.82 | 0.45 |
| 25:YA:1921:G:H2' | 25:YA:1922:G:H8 | 1.82 | 0.45 |
| 25:YA:2004:G:C4 | 25:YA:2005:A:C8 | 3.04 | 0.45 |
| 25:YA:2065:C:H2' | 25:YA:2066:C:H6 | 1.82 | 0.45 |
| 25:YA:2349:G:C6 | 25:YA:2369:A:C6 | 3.04 | 0.45 |
| 25:YA:2540:C:H2' | 25:YA:2541:A:O4' | 2.17 | 0.45 |
| 25:YA:265:A:N6 | 25:YA:428:A:C8 | 2.85 | 0.45 |
| 25:YA:557:U:H2' | 25:YA:558:G:C8 | 2.51 | 0.45 |
| 27:YD:18:VAL:HA | 27:YD:211:ARG:HH22 | 1.82 | 0.45 |
| 25:YA:1216:G:P | 40:YU:11:ARG:HH21 | 2.40 | 0.45 |
| 1:QA:556:C:H2' | 1:QA:557:G:H8 | 1.81 | 0.45 |
| 3:QC:23:TYR:HB3 | 10:QJ:93:GLY:O | 2.16 | 0.45 |
| 16:QP:19:ILE:N | 16:QP:37:GLY:O | 2.50 | 0.45 |
| 53:R7:5:TRP:NE1 | 53:R7:7:PRO:HG3 | 2.31 | 0.45 |
| 25:RA:2108:C:O2 | 25:RA:2181:G:N2 | 2.35 | 0.45 |
| 25:RA:270(D):C:H2' | 25:RA:270(E):G:C8 | 2.50 | 0.45 |
| 25:RA:2857:G:N2 | 25:RA:2860:A:OP2 | 2.33 | 0.45 |
| 25:RA:458:G:N2 | 25:RA:470:A:OP2 | 2.50 | 0.45 |
| 25:RA:580:C:H2' | 25:RA:581:C:C6 | 2.52 | 0.45 |
| 25:RA:754:C:H2' | 25:RA:755:C:C6 | 2.52 | 0.45 |
| 33:RN:91:LEU:HD21 | 33:RN:98:VAL:HG11 | 1.98 | 0.45 |
| 25:RA:2880:C:O3' | 37:RR:90:ARG:NH1 | 2.50 | 0.45 |
| 42:RW:111:HIS:HD2 | 42:RW:113:LYS:H | 1.63 | 0.45 |
| 1:XA:1301:U:H2' | 1:XA:1301:U:O2 | 2.17 | 0.45 |
| 1:XA:1236:A:H4' | 1:XA:1304:G:H4' | 1.99 | 0.45 |
| 2:XB:84:GLU:OE2 | 2:XB:233:SER:OG | 2.32 | 0.45 |
| 11:XK:57:THR:HG22 | 11:XK:59:TYR:H | 1.82 | 0.45 |
| 17:XQ:40:LYS:HE2 | 17:XQ:42:TYR:HE1 | 1.82 | 0.45 |
| 25:YA:814:C:H1' | 25:YA:1226:G:N2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:1675:C:H2' | 25:YA:1676:A:O4' | 2.17 | 0.45 |
| 25:YA:1790:C:H2' | 25:YA:1791:A:C4 | 2.52 | 0.45 |
| 25:YA:2314:C:H2' | 25:YA:2315:G:C8 | 2.47 | 0.45 |
| 25:YA:2443:C:H2' | 25:YA:2444:G:C8 | 2.51 | 0.45 |
| 25:YA:659:C:H2' | 25:YA:660:G:H8 | 1.82 | 0.45 |
| 25:YA:71:A:N6 | 25:YA:114:U:H1' | 2.30 | 0.45 |
| 31:YH:9:ILE:HD13 | 31:YH:49:VAL:HG12 | 1.98 | 0.45 |
| 37:YR:26:LYS:HE2 | 37:YR:70:LEU:O | 2.16 | 0.45 |
| 38:YS:110:LEU:O | 38:YS:112:PHE:HD1 | 1.99 | 0.45 |
| 40:YU:92:ARG:NE | 41:YV:11:GLN:H | 2.14 | 0.45 |
| 45:YZ:6:LYS:O | 45:YZ:62:PRO:HD3 | 2.16 | 0.45 |
| 1:QA:1099:G:H5'' | 2:QB:96:ARG:CZ | 2.46 | 0.45 |
| 1:QA:1121:U:H2' | 1:QA:1122:U:C6 | 2.51 | 0.45 |
| 1:QA:1253:G:H2' | 1:QA:1254:C:H6 | 1.82 | 0.45 |
| 1:QA:1320:C:C2 | 19:QS:72:GLY:HA3 | 2.51 | 0.45 |
| 1:QA:488:C:H2' | 1:QA:489:C:C6 | 2.51 | 0.45 |
| 3:QC:23:TYR:CD2 | 10:QJ:95:GLU:HB2 | 2.52 | 0.45 |
| 1:QA:1060:C:C5 | 3:QC:2:GLY:HA2 | 2.52 | 0.45 |
| 17:QQ:6:LEU:HD13 | 17:QQ:23:VAL:HG11 | 1.99 | 0.45 |
| 25:RA:1799:G:H4' | 25:RA:1800:C:O5' | 2.17 | 0.45 |
| 25:RA:1952:A:N3 | 25:RA:2560:C:O2' | 2.40 | 0.45 |
| 25:RA:2306:C:H2' | 25:RA:2307:G:H21 | 1.81 | 0.45 |
| 25:RA:2630:G:H2' | 25:RA:2631:G:C8 | 2.52 | 0.45 |
| 25:RA:2774:C:H2' | 25:RA:2775:A:O4' | 2.16 | 0.45 |
| 25:RA:541:C:H2' | 25:RA:542:C:H6 | 1.82 | 0.45 |
| 28:RE:74:PRO:HG2 | 28:RE:77:ILE:CG2 | 2.47 | 0.45 |
| 28:RE:78:LEU:HG | 28:RE:79:ARG:HG2 | 1.98 | 0.45 |
| 1:XA:178:C:C2 | 1:XA:179:A:C8 | 3.05 | 0.45 |
| 46:Y0:21:LEU:HD23 | 46:Y0:39:ARG:HG3 | 1.99 | 0.45 |
| 25:YA:1537:C:H2' | 25:YA:1538:G:C8 | 2.52 | 0.45 |
| 25:YA:2698:U:H2' | 25:YA:2699:C:H6 | 1.82 | 0.45 |
| 25:YA:273(C):C:H2' | 25:YA:273(D):C:C6 | 2.52 | 0.45 |
| 25:YA:534:U:H2' | 25:YA:535:C:C6 | 2.52 | 0.45 |
| 25:YA:709:U:H2' | 25:YA:710:G:C8 | 2.52 | 0.45 |
| 25:YA:724:U:H2' | 25:YA:725:G:O4' | 2.17 | 0.45 |
| 25:YA:874:G:H2' | 25:YA:875:G:H8 | 1.82 | 0.45 |
| 27:YD:151:LYS:O | 27:YD:154:LYS:NZ | 2.50 | 0.45 |
| 27:YD:143:HIS:HB2 | 27:YD:156:ALA:O | 2.17 | 0.45 |
| 31:YH:155:SER:OG | 55:Y9:17:ILE:HG21 | 2.17 | 0.45 |
| 31:YH:162:ILE:HG22 | 55:Y9:18:ARG:NH1 | 2.29 | 0.45 |
| 25:YA:1952:A:C6 | 34:YO:22:ILE:HD12 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:YP:47:ASP:OD1 | 35:YP:49:ARG:HG2 | 2.16 | 0.45 |
| 42:YW:57:ASN:O | 42:YW:61:ASN:HB2 | 2.17 | 0.45 |
| 1:QA:1133:G:H2' | 1:QA:1134:G:C8 | 2.52 | 0.45 |
| 1:QA:1225:A:H5'' | 1:QA:1226:C:OP2 | 2.16 | 0.45 |
| 1:QA:1253:G:H2' | 1:QA:1254:C:C6 | 2.52 | 0.45 |
| 1:QA:1288:A:H2' | 1:QA:1289:A:C8 | 2.52 | 0.45 |
| 1:QA:1318:A:O2' | 19:QS:37:ARG:HD3 | 2.17 | 0.45 |
| 1:QA:1330:U:H4' | 13:QM:23:TYR:CE1 | 2.52 | 0.45 |
| 1:QA:528:C:H41 | 12:QL:49:ASN:CG | 2.19 | 0.45 |
| 1:QA:608:A:H4' | 16:QP:32:TYR:OH | 2.17 | 0.45 |
| 1:QA:9:G:N7 | 1:QA:558:G:O2' | 2.50 | 0.45 |
| 6:QF:67:MET:HB2 | 6:QF:68:PRO:HD2 | 1.99 | 0.45 |
| 22:QW:32:G:H3' | 22:QW:33:C:O4' | 2.16 | 0.45 |
| 25:RA:172:C:H2' | 25:RA:173:G:C8 | 2.52 | 0.45 |
| 25:RA:2405:G:O2' | 25:RA:2406:U:OP2 | 2.32 | 0.45 |
| 25:RA:2845:G:H2' | 25:RA:2846:G:C8 | 2.51 | 0.45 |
| 25:RA:521:G:H2' | 25:RA:522:G:C8 | 2.51 | 0.45 |
| 26:RB:60:C:H2' | 26:RB:61:G:C8 | 2.52 | 0.45 |
| 29:RF:70:THR:HG23 | 29:RF:72:ARG:H | 1.80 | 0.45 |
| 25:RA:586:A:H4' | 29:RF:89:VAL:HG11 | 1.99 | 0.45 |
| 30:RG:173:LEU:HB3 | 30:RG:178:PHE:CD2 | 2.52 | 0.45 |
| 25:RA:995:C:O4' | 40:RU:57:PHE:HD2 | 2.00 | 0.45 |
| 1:XA:1404:C:H2' | 1:XA:1405:G:C8 | 2.52 | 0.45 |
| 1:XA:592:G:C6 | 1:XA:648:A:C6 | 3.04 | 0.45 |
| 1:XA:667:G:H4' | 15:XO:51:HIS:CE1 | 2.52 | 0.45 |
| 1:XA:707:C:OP1 | 11:XK:85:ARG:NH1 | 2.50 | 0.45 |
| 1:XA:714:G:H2' | 1:XA:715:A:H8 | 1.78 | 0.45 |
| 4:XD:112:VAL:HG12 | 4:XD:116:GLN:OE1 | 2.17 | 0.45 |
| 12:XL:84:LEU:HB2 | 12:XL:105:TYR:CE2 | 2.52 | 0.45 |
| 1:XA:323:U:H5'' | 20:XT:26:ASN:HD21 | 1.80 | 0.45 |
| 25:YA:1467:C:C5 | 25:YA:1546:C:H2' | 2.51 | 0.45 |
| 25:YA:2071:A:H2' | 25:YA:2072:G:C8 | 2.52 | 0.45 |
| 25:YA:218:A:C2 | 25:YA:235:U:H4' | 2.52 | 0.45 |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:H8 | 1.82 | 0.45 |
| 25:YA:796:C:H2' | 25:YA:797:C:C6 | 2.52 | 0.45 |
| 25:YA:911:A:H2' | 36:YQ:9:TYR:CE2 | 2.50 | 0.45 |
| 27:YD:96:HIS:ND1 | 27:YD:102:LYS:HG2 | 2.32 | 0.45 |
| 28:YE:60:ASN:CG | 28:YE:62:PRO:HD2 | 2.36 | 0.45 |
| 1:QA:1000:A:H2' | 1:QA:1001:G:H8 | 1.81 | 0.44 |
| 1:QA:1090:U:H2' | 1:QA:1091:U:C6 | 2.53 | 0.44 |
| 1:QA:1469:G:H2' | 1:QA:1470:G:C8 | 2.49 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:384:G:H2' | 1:QA:385:C:C6 | 2.52 | 0.44 |
| 1:QA:908:A:H2' | 1:QA:909:A:C8 | 2.52 | 0.44 |
| 5:QE:87:SER:HB3 | 5:QE:131:ILE:HD13 | 1.99 | 0.44 |
| 8:QH:104:ARG:HD2 | 8:QH:138:TRP:CE3 | 2.52 | 0.44 |
| 13:QM:14:ARG:HG2 | 13:QM:44:ARG:NH1 | 2.31 | 0.44 |
| 50:R4:61:ARG:HG2 | 50:R4:61:ARG:O | 2.16 | 0.44 |
| 25:RA:1657:C:H2' | 25:RA:1658:C:C6 | 2.52 | 0.44 |
| 25:RA:2294:C:H2' | 25:RA:2295:C:H6 | 1.82 | 0.44 |
| 25:RA:319:C:H2' | 25:RA:320:A:C8 | 2.51 | 0.44 |
| 25:RA:503:A:H4' | 25:RA:504:U:O5' | 2.17 | 0.44 |
| 26:RB:32:C:C2 | 26:RB:51:G:N2 | 2.85 | 0.44 |
| 25:RA:586:A:H5' | 29:RF:89:VAL:HG21 | 1.99 | 0.44 |
| 32:RI:14:ASP:O | 32:RI:16:GLY:N | 2.49 | 0.44 |
| 42:RW:110:LYS:HG3 | 42:RW:111:HIS:ND1 | 2.32 | 0.44 |
| 1:XA:1028(B):C:C4 | 1:XA:1029:G:H1' | 2.52 | 0.44 |
| 1:XA:163:C:H2' | 1:XA:164:U:C6 | 2.52 | 0.44 |
| 2:XB:141:GLU:O | 2:XB:144:ARG:HG3 | 2.17 | 0.44 |
| 4:XD:85:LYS:HD2 | 4:XD:92:VAL:HG11 | 1.99 | 0.44 |
| 1:XA:966:G:C2 | 22:XV:35:C:H5' | 2.52 | 0.44 |
| 25:YA:1628:G:H2' | 25:YA:1629:U:C6 | 2.52 | 0.44 |
| 25:YA:2564:A:C8 | 25:YA:2648:C:H5' | 2.52 | 0.44 |
| 25:YA:2683:C:O2 | 34:YO:70:LYS:HE3 | 2.17 | 0.44 |
| 25:YA:2692:C:H2' | 25:YA:2693:A:C8 | 2.52 | 0.44 |
| 25:YA:30:G:H2' | 25:YA:31:C:H6 | 1.82 | 0.44 |
| 25:YA:512:G:HO2' | 25:YA:513:A:H8 | 1.65 | 0.44 |
| 28:YE:11:MET:HG2 | 28:YE:24:THR:OG1 | 2.17 | 0.44 |
| 29:YF:73:ALA:HB3 | 29:YF:75:HIS:CE1 | 2.53 | 0.44 |
| 32:YI:80:PRO:HB2 | 32:YI:146:ALA:HB2 | 2.00 | 0.44 |
| 33:YN:12:ARG:NH1 | 33:YN:14:VAL:HG22 | 2.32 | 0.44 |
| 41:YV:75:PHE:HE1 | 41:YV:82:ARG:HE | 1.64 | 0.44 |
| 1:QA:1070:U:H2' | 1:QA:1071:C:C6 | 2.53 | 0.44 |
| 1:QA:1203:C:H2' | 1:QA:1204:A:H8 | 1.81 | 0.44 |
| 1:QA:1267:C:O2 | 21:QU:20:LYS:HD2 | 2.17 | 0.44 |
| 1:QA:1286:A:H2' | 1:QA:1287:A:H4' | 1.98 | 0.44 |
| 1:QA:1301:U:O2 | 1:QA:1301:U:H2' | 2.17 | 0.44 |
| 1:QA:867:G:O2' | 1:QA:873:A:N6 | 2.50 | 0.44 |
| 7:QG:75:VAL:HG12 | 7:QG:88:PRO:HB3 | 2.00 | 0.44 |
| 1:QA:1367:C:H5' | 10:QJ:60:ARG:NH1 | 2.32 | 0.44 |
| 13:QM:49:THR:HB | 13:QM:52:GLU:HG3 | 1.98 | 0.44 |
| 25:RA:1062:G:OP1 | 25:RA:1070:A:H4' | 2.17 | 0.44 |
| 25:RA:1141:U:O2' | 25:RA:1142(A):A:N7 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1811:G:H2' | 25:RA:1812:A:C8 | 2.51 | 0.44 |
| 25:RA:1825:A:H2' | 25:RA:1826:G:C8 | 2.52 | 0.44 |
| 25:RA:1946:U:H2' | 25:RA:1947:C:H6 | 1.83 | 0.44 |
| 25:RA:270(F):U:H2' | 25:RA:270(G):C:C6 | 2.53 | 0.44 |
| 25:RA:2712:U:HO2' | 25:RA:2712(A):A:P | 2.41 | 0.44 |
| 25:RA:2790:A:H2' | 25:RA:2791:C:H5'' | 1.99 | 0.44 |
| 25:RA:519:U:H2' | 25:RA:520:G:C8 | 2.52 | 0.44 |
| 25:RA:588:U:H2' | 25:RA:589:C:C6 | 2.52 | 0.44 |
| 27:RD:247:ALA:HA | 27:RD:253:GLN:HA | 1.99 | 0.44 |
| 25:RA:2224:G:OP1 | 27:RD:268:ARG:HD3 | 2.17 | 0.44 |
| 25:RA:2730:C:O2' | 28:RE:168:MET:O | 2.30 | 0.44 |
| 28:RE:13:ARG:HA | 28:RE:22:PRO:HA | 1.97 | 0.44 |
| 36:RQ:30:GLY:HA3 | 36:RQ:107:ALA:HB2 | 1.99 | 0.44 |
| 42:RW:64:MET:HB3 | 42:RW:69:LEU:HD21 | 1.99 | 0.44 |
| 1:XA:1355:G:H2' | 1:XA:1356:G:H8 | 1.82 | 0.44 |
| 1:XA:150:C:H2' | 1:XA:151:A:O4' | 2.17 | 0.44 |
| 1:XA:160:A:H2' | 1:XA:161:A:O4' | 2.18 | 0.44 |
| 1:XA:129(A):G:N1 | 1:XA:188:U:H4' | 2.33 | 0.44 |
| 1:XA:688:G:H2' | 1:XA:689:C:H6 | 1.82 | 0.44 |
| 7:XG:87:VAL:HG13 | 7:XG:152:ALA:HA | 2.00 | 0.44 |
| 9:XI:85:LEU:HD11 | 9:XI:96:LEU:HD21 | 1.99 | 0.44 |
| 20:XT:72:LEU:O | 20:XT:72:LEU:HD23 | 2.17 | 0.44 |
| 25:YA:2743:C:O5' | 55:Y9:25:VAL:HA | 2.17 | 0.44 |
| 55:Y9:26:ILE:HG13 | 55:Y9:26:ILE:O | 2.17 | 0.44 |
| 25:YA:2755:C:C5 | 55:Y9:3:VAL:HA | 2.52 | 0.44 |
| 25:YA:1527:G:H22 | 25:YA:1545:A:H3' | 1.81 | 0.44 |
| 25:YA:210:C:H2' | 25:YA:211:A:H8 | 1.83 | 0.44 |
| 25:YA:2712:U:C5 | 25:YA:2713:A:H5'' | 2.52 | 0.44 |
| 25:YA:524:U:H2' | 25:YA:525:U:C6 | 2.52 | 0.44 |
| 25:YA:638:G:H2' | 25:YA:639:U:H6 | 1.81 | 0.44 |
| 26:YB:43:C:O2' | 30:YG:98:ARG:NH2 | 2.49 | 0.44 |
| 30:YG:27:ASN:OD1 | 30:YG:28:VAL:N | 2.50 | 0.44 |
| 33:YN:123:TYR:HE2 | 33:YN:129:PRO:HD2 | 1.82 | 0.44 |
| 38:YS:39:ILE:HB | 38:YS:49:VAL:HB | 1.99 | 0.44 |
| 37:YR:103:ARG:NH1 | 42:YW:40:ASN:OD1 | 2.41 | 0.44 |
| 1:QA:113:G:H2' | 1:QA:114:U:H6 | 1.83 | 0.44 |
| 1:QA:115:G:H4' | 1:QA:116:A:O5' | 2.17 | 0.44 |
| 1:QA:1238:A:H62 | 1:QA:1299:A:N6 | 2.15 | 0.44 |
| 1:QA:189:U:O2 | 17:QQ:63:ARG:NH2 | 2.50 | 0.44 |
| 16:QP:2:VAL:HG13 | 16:QP:64:ALA:HA | 2.00 | 0.44 |
| 17:QQ:28:PRO:HA | 17:QQ:35:VAL:HA | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1212:G:H1' | 25:RA:1237:A:N6 | 2.32 | 0.44 |
| 25:RA:1278:A:H2' | 25:RA:1279:G:H8 | 1.81 | 0.44 |
| 25:RA:2231:C:H2' | 25:RA:2232:U:O4' | 2.17 | 0.44 |
| 25:RA:2702:U:H3 | 25:RA:2705:A:H61 | 1.66 | 0.44 |
| 25:RA:2845:G:H2' | 25:RA:2846:G:H8 | 1.83 | 0.44 |
| 1:XA:135:C:H2' | 1:XA:136:C:H5' | 1.99 | 0.44 |
| 1:XA:575:G:O2' | 1:XA:821:G:H5' | 2.17 | 0.44 |
| 1:XA:67:C:H2' | 1:XA:68:G:C8 | 2.53 | 0.44 |
| 1:XA:908:A:H2' | 1:XA:909:A:C8 | 2.52 | 0.44 |
| 1:XA:913:A:OP1 | 12:XL:46:LYS:NZ | 2.51 | 0.44 |
| 8:XH:20:TYR:HE2 | 8:XH:75:ARG:HD2 | 1.82 | 0.44 |
| 51:Y5:20:ARG:HA | 51:Y5:23:HIS:ND1 | 2.33 | 0.44 |
| 25:YA:2744:G:H5' | 55:Y9:24:TYR:CD2 | 2.52 | 0.44 |
| 25:YA:2742:C:C2 | 55:Y9:26:ILE:HG22 | 2.52 | 0.44 |
| 55:Y9:27:CYS:HB3 | 55:Y9:28:GLU:H | 1.59 | 0.44 |
| 25:YA:1297:C:H2' | 25:YA:1298:C:H6 | 1.81 | 0.44 |
| 25:YA:1317:A:H2' | 25:YA:1318:C:C6 | 2.52 | 0.44 |
| 25:YA:2133:G:H1' | 25:YA:2158:A:H61 | 1.82 | 0.44 |
| 25:YA:29:U:H2' | 25:YA:30:G:C8 | 2.52 | 0.44 |
| 25:YA:571:A:O2' | 41:YV:78:LYS:HE2 | 2.17 | 0.44 |
| 25:YA:898:C:H3' | 25:YA:899:A:H8 | 1.81 | 0.44 |
| 25:YA:974(A):C:H4' | 25:YA:975:G:O5' | 2.16 | 0.44 |
| 26:YB:30:C:H2' | 26:YB:31:C:O4' | 2.17 | 0.44 |
| 25:YA:1971:A:C8 | 27:YD:241:PRO:HB3 | 2.53 | 0.44 |
| 25:YA:1657:C:H4' | 28:YE:133:LYS:HB3 | 1.99 | 0.44 |
| 30:YG:173:LEU:HB3 | 30:YG:178:PHE:CD2 | 2.53 | 0.44 |
| 36:YQ:73:PRO:HA | 36:YQ:93:TYR:CD1 | 2.52 | 0.44 |
| 25:YA:1252:G:N2 | 40:YU:33:ARG:HB3 | 2.32 | 0.44 |
| 1:QA:1427:U:H2' | 1:QA:1428:A:C8 | 2.53 | 0.44 |
| 1:QA:1496:C:H2' | 1:QA:1497:G:C8 | 2.52 | 0.44 |
| 1:QA:1512:U:H2' | 1:QA:1513:A:C8 | 2.52 | 0.44 |
| 4:QD:93:PHE:CE2 | 4:QD:97:LEU:HD11 | 2.53 | 0.44 |
| 13:QM:86:CYS:SG | 13:QM:88:ARG:HG2 | 2.58 | 0.44 |
| 25:RA:2336:A:H61 | 46:R0:43:THR:HG21 | 1.83 | 0.44 |
| 49:R3:10:LYS:HB3 | 49:R3:53:LEU:HD23 | 1.98 | 0.44 |
| 25:RA:1321:A:C4 | 25:RA:1322:A:C8 | 3.05 | 0.44 |
| 25:RA:140:A:H8 | 25:RA:1408:C:O2' | 1.95 | 0.44 |
| 25:RA:1853:A:N6 | 25:RA:1889:A:N7 | 2.66 | 0.44 |
| 25:RA:2567:G:H2' | 25:RA:2568:C:H6 | 1.82 | 0.44 |
| 25:RA:2784:C:H2' | 25:RA:2785:C:C6 | 2.51 | 0.44 |
| 25:RA:414:C:H2' | 25:RA:415:A:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:554:U:H2' | 25:RA:556:G:C8 | 2.52 | 0.44 |
| 25:RA:924:C:H2' | 25:RA:925:C:C6 | 2.52 | 0.44 |
| 27:RD:69:ARG:HH21 | 27:RD:130:ALA:N | 2.16 | 0.44 |
| 25:RA:618(A):C:OP2 | 29:RF:103:LYS:HE3 | 2.16 | 0.44 |
| 29:RF:8:GLN:HG2 | 29:RF:8:GLN:O | 2.17 | 0.44 |
| 36:RQ:58:PHE:HD2 | 36:RQ:61:GLY:HA3 | 1.83 | 0.44 |
| 40:RU:108:GLU:HG3 | 41:RV:45:THR:OG1 | 2.17 | 0.44 |
| 43:RX:21:PHE:HE1 | 43:RX:92:LEU:HB3 | 1.81 | 0.44 |
| 1:XA:1127:G:H1' | 1:XA:1147:C:H42 | 1.82 | 0.44 |
| 1:XA:1064:G:H21 | 1:XA:1190:G:H2' | 1.82 | 0.44 |
| 1:XA:156:G:H2' | 1:XA:157:G:H8 | 1.82 | 0.44 |
| 1:XA:262:A:H2' | 1:XA:263:A:C8 | 2.52 | 0.44 |
| 1:XA:397:A:H5' | 1:XA:398:C:OP1 | 2.18 | 0.44 |
| 1:XA:877:C:H2' | 1:XA:878:G:C8 | 2.49 | 0.44 |
| 2:XB:163:PHE:HA | 2:XB:185:ILE:O | 2.18 | 0.44 |
| 9:XI:8:GLY:HA2 | 9:XI:79:LEU:HD12 | 1.99 | 0.44 |
| 13:XM:49:THR:HB | 13:XM:52:GLU:HG3 | 2.00 | 0.44 |
| 13:XM:4:ILE:H | 13:XM:9:ILE:HG22 | 1.82 | 0.44 |
| 14:XN:26:ARG:HD3 | 14:XN:43:CYS:HB3 | 1.99 | 0.44 |
| 17:XQ:12:SER:HB3 | 17:XQ:20:THR:HB | 2.00 | 0.44 |
| 11:XK:109:VAL:HG11 | 18:XR:84:LYS:HD2 | 2.00 | 0.44 |
| 22:XW:9:G:H5'' | 22:XW:10:G:OP2 | 2.17 | 0.44 |
| 25:YA:857:C:H4' | 46:Y0:23:VAL:HG21 | 2.00 | 0.44 |
| 25:YA:2743:C:OP2 | 55:Y9:25:VAL:HB | 2.17 | 0.44 |
| 55:Y9:27:CYS:C | 55:Y9:29:ASN:H | 2.20 | 0.44 |
| 25:YA:1048:A:P | 25:YA:1110:G:H22 | 2.41 | 0.44 |
| 25:YA:1345:C:H2' | 25:YA:1346:G:H8 | 1.81 | 0.44 |
| 25:YA:1562:A:H2' | 25:YA:1563:G:H8 | 1.83 | 0.44 |
| 25:YA:1756:G:H4' | 25:YA:1758:G:O4' | 2.18 | 0.44 |
| 25:YA:1790:C:H2' | 25:YA:1791:A:C5 | 2.52 | 0.44 |
| 25:YA:395:U:H2' | 25:YA:396:G:C8 | 2.52 | 0.44 |
| 25:YA:635:C:O2' | 25:YA:639:U:OP1 | 2.35 | 0.44 |
| 25:YA:753:C:H2' | 25:YA:754:C:H6 | 1.82 | 0.44 |
| 25:YA:934:G:H2' | 25:YA:935:C:H6 | 1.83 | 0.44 |
| 27:YD:69:ARG:HH21 | 27:YD:130:ALA:HB2 | 1.82 | 0.44 |
| 39:YT:36:GLU:HG3 | 39:YT:41:ARG:HE | 1.81 | 0.44 |
| 1:QA:1095:U:P | 1:QA:1108:G:H1 | 2.40 | 0.44 |
| 1:QA:1348:U:C4 | 1:QA:1374:A:H2 | 2.35 | 0.44 |
| 4:QD:22:LYS:HD3 | 57:QD:301:SF4:S3 | 2.58 | 0.44 |
| 11:QK:20:TYR:HE1 | 11:QK:83:ILE:HD12 | 1.81 | 0.44 |
| 12:QL:32:PHE:HB3 | 12:QL:84:LEU:HD11 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:QS:22:LEU:HD21 | 19:QS:29:ARG:N | 2.32 | 0.44 |
| 53:R7:30:VAL:HG22 | 53:R7:33:ARG:HH21 | 1.82 | 0.44 |
| 25:RA:1542:G:H5'' | 25:RA:1543:A:OP2 | 2.18 | 0.44 |
| 25:RA:1657:C:H2' | 25:RA:1658:C:H6 | 1.82 | 0.44 |
| 27:RD:142:VAL:HG23 | 27:RD:193:VAL:HA | 1.98 | 0.44 |
| 29:RF:156:LEU:HD21 | 29:RF:163:VAL:HG12 | 1.99 | 0.44 |
| 25:RA:2531:A:N7 | 31:RH:175:LYS:HD2 | 2.33 | 0.44 |
| 33:RN:35:ARG:HB2 | 33:RN:42:TRP:HH2 | 1.82 | 0.44 |
| 35:RP:85:LEU:HD23 | 35:RP:88:LEU:HD21 | 1.99 | 0.44 |
| 40:RU:91:ASP:HA | 40:RU:95:LEU:HB2 | 1.99 | 0.44 |
| 1:XA:1320:C:H2' | 1:XA:1321:C:C6 | 2.52 | 0.44 |
| 1:XA:1329:A:H5'' | 13:XM:26:GLY:N | 2.32 | 0.44 |
| 1:XA:1499:A:H1' | 1:XA:1520:G:H5' | 1.98 | 0.44 |
| 1:XA:163:C:H2' | 1:XA:164:U:H6 | 1.81 | 0.44 |
| 1:XA:246:A:C2 | 1:XA:282:A:C5 | 3.05 | 0.44 |
| 1:XA:674:G:H1' | 18:XR:81:PHE:HE2 | 1.83 | 0.44 |
| 1:XA:925:G:C2 | 1:XA:927:G:C8 | 3.06 | 0.44 |
| 9:XI:42:ARG:NH2 | 9:XI:75:ASP:OD1 | 2.43 | 0.44 |
| 12:XL:53:ARG:HH12 | 12:XL:92:ASP:HB2 | 1.82 | 0.44 |
| 13:XM:108:ARG:NH2 | 13:XM:111:LYS:HD3 | 2.32 | 0.44 |
| 17:XQ:51:TYR:HE2 | 17:XQ:73:VAL:HG11 | 1.81 | 0.44 |
| 25:YA:20:C:N3 | 25:YA:520:G:N1 | 2.38 | 0.44 |
| 25:YA:2525:G:H21 | 55:Y9:28:GLU:CG | 2.17 | 0.44 |
| 25:YA:2527:C:C4 | 25:YA:2528:U:C4 | 3.06 | 0.44 |
| 25:YA:363(A):A:H2' | 25:YA:363(B):G:H8 | 1.82 | 0.44 |
| 25:YA:851:U:H2' | 25:YA:852:G:H8 | 1.82 | 0.44 |
| 25:YA:870:A:OP1 | 36:YQ:6:ARG:NH2 | 2.40 | 0.44 |
| 25:YA:983:A:H2' | 25:YA:984:A:C8 | 2.52 | 0.44 |
| 25:YA:616:A:H4' | 29:YF:182:ASN:ND2 | 2.31 | 0.44 |
| 30:YG:126:ASP:OD2 | 30:YG:130:ASN:HB2 | 2.18 | 0.44 |
| 30:YG:5:VAL:HG12 | 30:YG:8:LYS:H | 1.82 | 0.44 |
| 30:YG:60:LEU:HD22 | 30:YG:68:PRO:HB3 | 2.00 | 0.44 |
| 34:YO:64:ARG:HH12 | 39:YT:70:VAL:HG21 | 1.82 | 0.44 |
| 37:YR:91:GLN:O | 37:YR:91:GLN:HG2 | 2.16 | 0.44 |
| 41:YV:4:ILE:HG13 | 41:YV:40:LEU:HD12 | 1.99 | 0.44 |
| 1:QA:1121:U:C2 | 1:QA:1122:U:C5 | 3.05 | 0.44 |
| 1:QA:1422:G:H2' | 1:QA:1423:G:H8 | 1.83 | 0.44 |
| 1:QA:1511:G:H2' | 1:QA:1512:U:O4' | 2.16 | 0.44 |
| 2:QB:88:ALA:HB2 | 2:QB:219:VAL:HG13 | 2.00 | 0.44 |
| 4:QD:142:PRO:HA | 4:QD:185:PHE:HD2 | 1.81 | 0.44 |
| 5:QE:15:ARG:HD2 | 5:QE:26:PHE:CD2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:686:U:H1' | 11:QK:42:TRP:HE1 | 1.82 | 0.44 |
| 25:RA:1811:G:H2' | 25:RA:1812:A:H8 | 1.83 | 0.44 |
| 25:RA:2494:G:OP1 | 46:R0:3:HIS:N | 2.50 | 0.44 |
| 25:RA:520:G:H2' | 25:RA:521:G:C8 | 2.52 | 0.44 |
| 38:RS:11:LYS:O | 38:RS:15:ARG:HB2 | 2.18 | 0.44 |
| 1:XA:1219:U:OP1 | 14:XN:19:ARG:NH2 | 2.40 | 0.44 |
| 1:XA:560:U:H5' | 1:XA:566:G:N2 | 2.33 | 0.44 |
| 5:XE:153:LYS:HG3 | 5:XE:155:GLU:H | 1.83 | 0.44 |
| 17:XQ:42:TYR:HD2 | 17:XQ:59:ILE:HD11 | 1.82 | 0.44 |
| 48:Y2:25:VAL:O | 48:Y2:29:LYS:HG2 | 2.17 | 0.44 |
| 25:YA:1412:A:H2' | 25:YA:1413:G:C8 | 2.52 | 0.44 |
| 25:YA:1907:G:O6 | 25:YA:1924:C:N4 | 2.51 | 0.44 |
| 25:YA:2507:C:H2' | 25:YA:2508:G:O4' | 2.18 | 0.44 |
| 25:YA:2532:G:N2 | 25:YA:2663:G:O2' | 2.50 | 0.44 |
| 25:YA:2712:U:H5 | 25:YA:2713:A:H5'' | 1.82 | 0.44 |
| 25:YA:704:G:H1' | 25:YA:727:A:H61 | 1.83 | 0.44 |
| 25:YA:760:G:H2' | 25:YA:761:A:O4' | 2.16 | 0.44 |
| 25:YA:834:C:H2' | 25:YA:835:A:H8 | 1.82 | 0.44 |
| 36:YQ:36:ALA:HB1 | 36:YQ:127:ILE:HD12 | 1.99 | 0.44 |
| 25:YA:1252:G:N2 | 40:YU:37:GLU:OE2 | 2.42 | 0.44 |
| 1:QA:1145:C:H4' | 1:QA:1146:A:C8 | 2.52 | 0.44 |
| 1:QA:1313:U:H2' | 1:QA:1314:C:C6 | 2.53 | 0.44 |
| 1:QA:221:C:C2 | 1:QA:222:U:C5 | 3.06 | 0.44 |
| 1:QA:269:C:H2' | 1:QA:270:A:C8 | 2.52 | 0.44 |
| 1:QA:593:G:H1 | 1:QA:646:U:H3 | 1.66 | 0.44 |
| 1:QA:998(A):C:H2' | 1:QA:999:U:C6 | 2.53 | 0.44 |
| 6:QF:97:PHE:HD2 | 18:QR:31:LEU:HD21 | 1.83 | 0.44 |
| 21:QU:6:ARG:HE | 21:QU:15:ARG:NH2 | 2.15 | 0.44 |
| 25:RA:1499:C:H2' | 25:RA:1500:G:H8 | 1.83 | 0.44 |
| 25:RA:2557:G:H2' | 25:RA:2558:C:C6 | 2.52 | 0.44 |
| 25:RA:2574:G:H2' | 25:RA:2575:C:O4' | 2.17 | 0.44 |
| 25:RA:2648:C:H2' | 25:RA:2649:U:C6 | 2.53 | 0.44 |
| 25:RA:2649:U:H2' | 25:RA:2650:U:C6 | 2.52 | 0.44 |
| 25:RA:2788:C:O2' | 25:RA:2809:A:N3 | 2.46 | 0.44 |
| 27:RD:94:LEU:HD13 | 27:RD:104:TYR:CE1 | 2.47 | 0.44 |
| 29:RF:113:ALA:HB1 | 29:RF:186:ILE:HG21 | 1.98 | 0.44 |
| 39:RT:120:ARG:O | 39:RT:123:GLN:HB2 | 2.17 | 0.44 |
| 25:RA:996:A:H4' | 40:RU:92:ARG:CG | 2.48 | 0.44 |
| 40:RU:92:ARG:NE | 41:RV:11:GLN:H | 2.16 | 0.44 |
| 1:XA:279:A:OP1 | 1:XA:280:C:O2' | 2.26 | 0.44 |
| 1:XA:505:G:H2' | 1:XA:506:G:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:XR:53:ARG:HH21 | 18:XR:59:SER:HA | 1.82 | 0.44 |
| 50:Y4:51:ASP:OD1 | 50:Y4:52:THR:N | 2.46 | 0.44 |
| 25:YA:1782:C:H1' | 25:YA:2609:U:H5'' | 2.00 | 0.44 |
| 25:YA:2018:G:H2' | 25:YA:2019:A:H8 | 1.83 | 0.44 |
| 25:YA:2290:G:H2' | 25:YA:2291:U:H6 | 1.83 | 0.44 |
| 25:YA:2695:C:H2' | 25:YA:2696:U:H6 | 1.82 | 0.44 |
| 25:YA:2838:G:C4 | 25:YA:2839:G:C8 | 3.06 | 0.44 |
| 25:YA:775:G:C5 | 25:YA:794:G:C8 | 3.05 | 0.44 |
| 25:YA:845:G:OP2 | 25:YA:845:G:H8 | 1.99 | 0.44 |
| 26:YB:40:U:H1' | 26:YB:45:A:H61 | 1.82 | 0.44 |
| 27:YD:30:GLU:CD | 27:YD:63:ARG:HE | 2.21 | 0.44 |
| 31:YH:137:ASP:CG | 31:YH:138:LYS:H | 2.21 | 0.44 |
| 28:YE:152:LYS:HG3 | 33:YN:78:TYR:CE1 | 2.53 | 0.44 |
| 1:QA:1391:U:H2' | 1:QA:1392:G:H8 | 1.83 | 0.44 |
| 1:QA:1427:U:H2' | 1:QA:1428:A:H8 | 1.82 | 0.44 |
| 1:QA:264:U:H2' | 1:QA:265:G:O4' | 2.18 | 0.44 |
| 1:QA:328:C:H4' | 1:QA:329:A:O5' | 2.18 | 0.44 |
| 1:QA:770:C:H2' | 1:QA:771:G:H8 | 1.81 | 0.44 |
| 2:QB:24:TRP:HB2 | 2:QB:190:THR:HB | 2.00 | 0.44 |
| 8:QH:14:ARG:O | 8:QH:18:ARG:HG2 | 2.17 | 0.44 |
| 13:QM:87:TYR:O | 13:QM:91:ARG:HG2 | 2.18 | 0.44 |
| 25:RA:1059:G:OP2 | 25:RA:1060:U:H5'' | 2.18 | 0.44 |
| 25:RA:1628:G:H2' | 25:RA:1629:U:C6 | 2.52 | 0.44 |
| 25:RA:1856:G:N1 | 25:RA:1887:C:N3 | 2.65 | 0.44 |
| 25:RA:2364:C:H2' | 25:RA:2365:G:O4' | 2.17 | 0.44 |
| 25:RA:2596:U:H2' | 25:RA:2597:G:O4' | 2.18 | 0.44 |
| 25:RA:2695:C:H2' | 25:RA:2696:U:C6 | 2.53 | 0.44 |
| 25:RA:553:U:H2' | 25:RA:554:U:O4' | 2.18 | 0.44 |
| 25:RA:606:U:H4' | 25:RA:658:C:H4' | 2.00 | 0.44 |
| 25:RA:78:A:H2' | 25:RA:79:G:C8 | 2.51 | 0.44 |
| 25:RA:823:G:H2' | 25:RA:824:A:H8 | 1.83 | 0.44 |
| 27:RD:124:PRO:O | 27:RD:129:ASN:ND2 | 2.51 | 0.44 |
| 28:RE:32:PRO:HA | 28:RE:90:THR:HA | 1.99 | 0.44 |
| 1:XA:1352:C:H2' | 1:XA:1353:G:C8 | 2.53 | 0.44 |
| 1:XA:152:A:H62 | 1:XA:169:C:N4 | 2.16 | 0.44 |
| 1:XA:186:C:H2' | 1:XA:186(A):C:C6 | 2.52 | 0.44 |
| 1:XA:271:C:H2' | 1:XA:272:C:H6 | 1.83 | 0.44 |
| 1:XA:402:G:OP1 | 4:XD:74:GLN:HG2 | 2.18 | 0.44 |
| 1:XA:893:C:C2 | 1:XA:894:G:C8 | 3.06 | 0.44 |
| 12:XL:33:ARG:HG2 | 12:XL:60:LEU:HD13 | 2.00 | 0.44 |
| 1:XA:1318:A:O2' | 19:XS:37:ARG:HD2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:131:G:H2' | 25:YA:132:G:H8 | 1.82 | 0.44 |
| 25:YA:1604:C:H2' | 25:YA:1605:C:H6 | 1.83 | 0.44 |
| 25:YA:1761:C:H42 | 25:YA:1762:A:H62 | 1.66 | 0.44 |
| 25:YA:2174:C:H2' | 25:YA:2175:C:C6 | 2.53 | 0.44 |
| 25:YA:2505:G:H2' | 25:YA:2576:G:H1 | 1.83 | 0.44 |
| 25:YA:2785:C:H2' | 25:YA:2786:U:H6 | 1.81 | 0.44 |
| 26:YB:32:C:C2 | 26:YB:51:G:N2 | 2.85 | 0.44 |
| 28:YE:120:TRP:CD1 | 28:YE:155:LYS:HB3 | 2.53 | 0.44 |
| 42:YW:22:ASP:OD1 | 42:YW:25:ARG:NH1 | 2.48 | 0.44 |
| 43:YX:5:TYR:CE2 | 48:Y2:30:ARG:HB2 | 2.53 | 0.44 |
| 1:QA:1040:U:H2' | 1:QA:1041:A:C8 | 2.53 | 0.44 |
| 1:QA:1200:C:H4' | 1:QA:1201:A:H5' | 2.00 | 0.44 |
| 1:QA:1461:G:H2' | 1:QA:1462:G:H8 | 1.83 | 0.44 |
| 1:QA:412:A:H4' | 1:QA:413:G:O5' | 2.16 | 0.44 |
| 1:QA:456:C:H2' | 1:QA:457:C:C6 | 2.52 | 0.44 |
| 1:QA:539:A:H2' | 1:QA:540:G:H8 | 1.82 | 0.44 |
| 1:QA:552:U:H2' | 1:QA:553:A:C8 | 2.52 | 0.44 |
| 4:QD:105:VAL:HG13 | 4:QD:110:PHE:HB2 | 2.00 | 0.44 |
| 4:QD:57:ARG:HB3 | 4:QD:206:PHE:CD1 | 2.53 | 0.44 |
| 1:QA:1291:G:H5'' | 7:QG:41:ARG:HH21 | 1.83 | 0.44 |
| 1:QA:1367:C:OP2 | 9:QI:112:LYS:NZ | 2.51 | 0.44 |
| 20:QT:72:LEU:O | 20:QT:72:LEU:HD23 | 2.18 | 0.44 |
| 22:QW:10:G:H2' | 22:QW:11:A:C8 | 2.52 | 0.44 |
| 25:RA:2355:C:H1' | 46:R0:39:ARG:HH21 | 1.82 | 0.44 |
| 51:R5:20:ARG:HA | 51:R5:23:HIS:ND1 | 2.33 | 0.44 |
| 25:RA:1137:G:H2' | 25:RA:1138:G:C8 | 2.53 | 0.44 |
| 25:RA:1418:G:N2 | 25:RA:1581:G:O6 | 2.51 | 0.44 |
| 25:RA:1459:G:C5 | 25:RA:1461:G:C8 | 3.05 | 0.44 |
| 25:RA:1605:C:H2' | 25:RA:1606:G:O4' | 2.18 | 0.44 |
| 25:RA:1656:C:H2' | 25:RA:1657:C:C6 | 2.51 | 0.44 |
| 25:RA:305:U:H2' | 25:RA:306:U:C6 | 2.53 | 0.44 |
| 25:RA:846:C:H42 | 25:RA:931:G:H1 | 1.65 | 0.44 |
| 25:RA:2392:A:H8 | 35:RP:60:MET:HG2 | 1.81 | 0.44 |
| 36:RQ:79:LEU:HB3 | 46:R0:5:LYS:HD3 | 1.99 | 0.44 |
| 38:RS:3:ARG:HD3 | 38:RS:4:LEU:HD13 | 2.00 | 0.44 |
| 39:RT:108:ARG:HG3 | 39:RT:111:ARG:NH2 | 2.33 | 0.44 |
| 43:RX:40:LYS:HG3 | 43:RX:51:VAL:HG11 | 2.00 | 0.44 |
| 1:XA:1014:A:C2 | 1:XA:1219:U:H1' | 2.53 | 0.44 |
| 1:XA:1267:C:O2 | 21:XU:20:LYS:HD2 | 2.18 | 0.44 |
| 1:XA:543:C:OP1 | 4:XD:14:ARG:HG3 | 2.18 | 0.44 |
| 1:XA:792:A:H1' | 1:XA:794:A:N7 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:857:C:H2' | 1:XA:858:G:O4' | 2.18 | 0.44 |
| 2:XB:61:LEU:HG | 2:XB:66:GLY:HA3 | 1.98 | 0.44 |
| 6:XF:49:ALA:HB1 | 18:XR:80:PRO:HB3 | 1.99 | 0.44 |
| 25:YA:1059:G:OP2 | 25:YA:1060:U:H5'' | 2.17 | 0.44 |
| 25:YA:1084:A:H5' | 25:YA:1085:A:OP2 | 2.18 | 0.44 |
| 25:YA:1338:G:O2' | 25:YA:1393:A:N1 | 2.43 | 0.44 |
| 25:YA:1400:G:H2' | 25:YA:1401:G:C8 | 2.52 | 0.44 |
| 25:YA:1505:C:H2' | 25:YA:1506:C:H6 | 1.82 | 0.44 |
| 25:YA:1534:G:N3 | 25:YA:1534:G:H2' | 2.33 | 0.44 |
| 25:YA:184:C:H2' | 25:YA:185:U:H6 | 1.83 | 0.44 |
| 25:YA:2001:A:H2' | 25:YA:2002:G:H8 | 1.82 | 0.44 |
| 25:YA:563:G:C6 | 25:YA:2018:G:C5 | 3.06 | 0.44 |
| 25:YA:2023:G:H4' | 25:YA:2617:C:O3' | 2.18 | 0.44 |
| 25:YA:2292:C:H2' | 25:YA:2293:C:C6 | 2.53 | 0.44 |
| 25:YA:852:G:H2' | 25:YA:853:G:C8 | 2.51 | 0.44 |
| 25:YA:971:C:O2' | 25:YA:983:A:N3 | 2.38 | 0.44 |
| 25:YA:1797:C:O2' | 27:YD:259:THR:HG22 | 2.17 | 0.44 |
| 29:YF:40:GLN:HE22 | 29:YF:182:ASN:HB2 | 1.83 | 0.44 |
| 32:YI:109:ILE:HB | 32:YI:130:TYR:CE1 | 2.53 | 0.44 |
| 1:QA:1129:C:H4' | 1:QA:1130:A:C8 | 2.52 | 0.43 |
| 1:QA:346:G:OP1 | 39:RT:41:ARG:NH1 | 2.51 | 0.43 |
| 1:QA:401:C:H2' | 1:QA:402:G:C8 | 2.53 | 0.43 |
| 1:QA:620:C:H2' | 1:QA:621:A:O4' | 2.18 | 0.43 |
| 1:QA:981:U:H5' | 14:QN:21:TYR:CZ | 2.52 | 0.43 |
| 15:QO:15:PHE:CE1 | 15:QO:84:LYS:HD3 | 2.53 | 0.43 |
| 18:QR:50:ILE:HG13 | 18:QR:74:ARG:HH22 | 1.82 | 0.43 |
| 49:R3:5:LYS:HD2 | 49:R3:34:GLU:OE2 | 2.18 | 0.43 |
| 25:RA:1295:C:H2' | 25:RA:1296:G:H8 | 1.82 | 0.43 |
| 25:RA:777:A:H2' | 25:RA:778:G:C8 | 2.53 | 0.43 |
| 27:RD:12:SER:HB2 | 27:RD:208:LYS:HB3 | 2.00 | 0.43 |
| 25:RA:1812:A:C4' | 27:RD:46:GLN:HE22 | 2.31 | 0.43 |
| 31:RH:88:LEU:HA | 31:RH:130:ARG:HA | 2.00 | 0.43 |
| 28:RE:19:ARG:HG3 | 34:RO:72:PRO:HB2 | 2.00 | 0.43 |
| 43:RX:34:ALA:O | 43:RX:77:LYS:NZ | 2.39 | 0.43 |
| 36:RQ:62:GLY:HA2 | 45:RZ:116:VAL:HG21 | 2.00 | 0.43 |
| 45:RZ:97:GLU:HG2 | 45:RZ:125:LEU:HD11 | 2.00 | 0.43 |
| 1:XA:1178:G:OP2 | 9:XI:93:ARG:NH2 | 2.50 | 0.43 |
| 1:XA:222:U:H2' | 1:XA:223:U:H6 | 1.82 | 0.43 |
| 1:XA:925:G:H1' | 1:XA:1502:A:C4 | 2.53 | 0.43 |
| 19:XS:10:PHE:CE2 | 19:XS:16:LEU:HB2 | 2.52 | 0.43 |
| 24:XY:41:C:H2' | 24:XY:42:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1357:U:H2' | 25:YA:1358:G:O4' | 2.17 | 0.43 |
| 25:YA:1639:U:H2' | 25:YA:1640:C:H5'' | 1.98 | 0.43 |
| 25:YA:1800:C:C6 | 25:YA:1802:A:H1' | 2.53 | 0.43 |
| 25:YA:2142:C:H2' | 25:YA:2143:C:C6 | 2.53 | 0.43 |
| 25:YA:2182:G:H2' | 25:YA:2183:C:C6 | 2.53 | 0.43 |
| 25:YA:513:A:H2 | 25:YA:582:G:H4' | 1.83 | 0.43 |
| 25:YA:942:G:H2' | 25:YA:943:U:O4' | 2.18 | 0.43 |
| 29:YF:8:GLN:HG2 | 29:YF:8:GLN:O | 2.18 | 0.43 |
| 34:YO:64:ARG:NH1 | 39:YT:70:VAL:HG21 | 2.33 | 0.43 |
| 1:QA:67:C:O2' | 1:QA:171:A:N3 | 2.41 | 0.43 |
| 1:QA:21:G:H21 | 1:QA:914:A:H62 | 1.66 | 0.43 |
| 1:QA:509:A:H4' | 1:QA:510:A:OP1 | 2.18 | 0.43 |
| 1:QA:543:C:OP2 | 4:QD:10:ARG:NH1 | 2.51 | 0.43 |
| 1:QA:731:G:OP1 | 1:QA:766:A:H1' | 2.18 | 0.43 |
| 1:QA:918:A:H2' | 1:QA:919:A:C8 | 2.53 | 0.43 |
| 1:QA:966:G:H2' | 1:QA:967:C:C6 | 2.53 | 0.43 |
| 1:QA:1112:C:H1' | 3:QC:179:ARG:NH1 | 2.33 | 0.43 |
| 9:QI:104:ARG:NH1 | 9:QI:105:ASP:O | 2.50 | 0.43 |
| 9:QI:5:TYR:CE1 | 9:QI:16:ARG:HB2 | 2.53 | 0.43 |
| 15:QO:87:ILE:HG22 | 15:QO:88:ARG:N | 2.30 | 0.43 |
| 52:R6:38:LYS:HB2 | 52:R6:49:HIS:CE1 | 2.53 | 0.43 |
| 54:R8:54:GLU:O | 54:R8:58:ILE:HG12 | 2.18 | 0.43 |
| 25:RA:1399:C:H2' | 25:RA:1400:G:C8 | 2.52 | 0.43 |
| 25:RA:1630:G:H2' | 25:RA:1630(A):C:C6 | 2.52 | 0.43 |
| 25:RA:2292:C:H2' | 25:RA:2293:C:C6 | 2.53 | 0.43 |
| 25:RA:2677:G:C6 | 25:RA:2731:G:C6 | 3.06 | 0.43 |
| 26:RB:74:U:H2' | 26:RB:75:G:O4' | 2.17 | 0.43 |
| 27:RD:72:LYS:HG3 | 27:RD:97:TYR:HE2 | 1.80 | 0.43 |
| 29:RF:178:PRO:HB3 | 29:RF:198:ALA:HB2 | 2.00 | 0.43 |
| 35:RP:47:ASP:OD1 | 35:RP:49:ARG:HG2 | 2.17 | 0.43 |
| 35:RP:84:ASN:OD1 | 35:RP:116:GLY:HA3 | 2.18 | 0.43 |
| 1:XA:105:G:H2' | 1:XA:106:C:C6 | 2.52 | 0.43 |
| 1:XA:790:A:H2' | 1:XA:791:G:C8 | 2.53 | 0.43 |
| 3:XC:19:GLU:O | 3:XC:40:ARG:NH2 | 2.51 | 0.43 |
| 4:XD:102:ASP:OD1 | 4:XD:103:ASN:N | 2.51 | 0.43 |
| 9:XI:63:ILE:HG21 | 9:XI:77:ILE:HG12 | 2.00 | 0.43 |
| 9:XI:79:LEU:HD11 | 9:XI:83:ARG:HE | 1.82 | 0.43 |
| 13:XM:40:ASN:HB3 | 13:XM:43:THR:HG23 | 1.99 | 0.43 |
| 50:Y4:55:ARG:O | 50:Y4:56:VAL:HG13 | 2.17 | 0.43 |
| 25:YA:1530:G:O6 | 25:YA:1542:G:N2 | 2.51 | 0.43 |
| 25:YA:1803:A:H2 | 25:YA:1823:G:O4' | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2537:U:H2' | 25:YA:2538:C:O4' | 2.19 | 0.43 |
| 25:YA:2547:U:H2' | 25:YA:2548:G:C8 | 2.53 | 0.43 |
| 25:YA:270(Y):G:O2' | 25:YA:270(Z):U:O4' | 2.28 | 0.43 |
| 25:YA:2761:G:C6 | 25:YA:2762:G:C4 | 3.06 | 0.43 |
| 25:YA:626:U:O4 | 35:YP:81:GLN:NE2 | 2.49 | 0.43 |
| 25:YA:742:G:H2' | 25:YA:743:G:C8 | 2.52 | 0.43 |
| 31:YH:149:ARG:HB3 | 55:Y9:20:HIS:HB2 | 2.00 | 0.43 |
| 34:YO:47:ILE:HG13 | 34:YO:48:PRO:HD2 | 1.99 | 0.43 |
| 34:YO:64:ARG:HB2 | 34:YO:83:ALA:HB3 | 1.99 | 0.43 |
| 36:YQ:116:GLU:O | 36:YQ:120:ILE:HG12 | 2.18 | 0.43 |
| 26:YB:30:C:OP2 | 38:YS:32:LEU:HD11 | 2.18 | 0.43 |
| 41:YV:51:VAL:HG12 | 41:YV:53:GLU:H | 1.83 | 0.43 |
| 43:YX:53:LYS:H | 43:YX:82:GLN:HB3 | 1.82 | 0.43 |
| 44:YY:20:TYR:CE2 | 44:YY:43:ASN:HA | 2.53 | 0.43 |
| 1:QA:538:G:H2' | 1:QA:539:A:C8 | 2.53 | 0.43 |
| 47:R1:52:ARG:HH11 | 47:R1:57:GLU:HB2 | 1.82 | 0.43 |
| 50:R4:51:ASP:OD1 | 50:R4:52:THR:N | 2.46 | 0.43 |
| 25:RA:1401:G:H2' | 25:RA:1402:C:C6 | 2.53 | 0.43 |
| 25:RA:1534:G:H2' | 25:RA:1534:G:N3 | 2.33 | 0.43 |
| 25:RA:172:C:H2' | 25:RA:173:G:H8 | 1.83 | 0.43 |
| 25:RA:1764:G:C6 | 25:RA:1989:G:N1 | 2.86 | 0.43 |
| 25:RA:189:G:H2' | 25:RA:205:G:N2 | 2.33 | 0.43 |
| 25:RA:2386:C:H2' | 25:RA:2387:U:C6 | 2.52 | 0.43 |
| 25:RA:2432:A:H2' | 25:RA:2433:A:C8 | 2.53 | 0.43 |
| 25:RA:820:A:H4' | 25:RA:836:G:N2 | 2.33 | 0.43 |
| 25:RA:923:C:H2' | 25:RA:924:C:C6 | 2.53 | 0.43 |
| 25:RA:846:C:N3 | 25:RA:930:U:N3 | 2.65 | 0.43 |
| 25:RA:2635:C:H5" | 28:RE:78:LEU:HA | 1.99 | 0.43 |
| 33:RN:67:LEU:O | 33:RN:88:GLU:HB2 | 2.19 | 0.43 |
| 39:RT:93:ARG:N | 39:RT:115:ARG:O | 2.36 | 0.43 |
| 40:RU:8:VAL:HG22 | 40:RU:12:ARG:HG3 | 1.99 | 0.43 |
| 45:RZ:149:SER:HB2 | 45:RZ:172:ALA:O | 2.17 | 0.43 |
| 45:RZ:54:HIS:HB3 | 45:RZ:101:PRO:HD3 | 2.01 | 0.43 |
| 45:RZ:59:LEU:O | 45:RZ:60:GLU:HG2 | 2.17 | 0.43 |
| 1:XA:173:U:H5" | 1:XA:197:A:O4' | 2.18 | 0.43 |
| 1:XA:757:U:H2' | 1:XA:758:G:O4' | 2.19 | 0.43 |
| 2:XB:115:LEU:HD13 | 2:XB:145:LEU:HB3 | 1.99 | 0.43 |
| 4:XD:142:PRO:HA | 4:XD:185:PHE:HD2 | 1.82 | 0.43 |
| 8:XH:121:ASP:OD1 | 8:XH:122:ARG:N | 2.51 | 0.43 |
| 25:YA:1157:G:O2' | 49:Y3:31:LEU:HD12 | 2.19 | 0.43 |
| 54:Y8:26:LYS:HD3 | 54:Y8:47:LYS:HB3 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1061:U:H3' | 25:YA:1062:G:C5' | 2.48 | 0.43 |
| 25:YA:1178:C:H2' | 25:YA:1179:C:C6 | 2.53 | 0.43 |
| 25:YA:1526:G:C6 | 25:YA:1527:G:C6 | 3.06 | 0.43 |
| 25:YA:2154:G:H2' | 25:YA:2155:G:C8 | 2.53 | 0.43 |
| 25:YA:2543:G:H2' | 25:YA:2544:G:H8 | 1.82 | 0.43 |
| 25:YA:2610:C:H4' | 25:YA:2611:U:H5' | 2.00 | 0.43 |
| 25:YA:2649:U:H2' | 25:YA:2650:U:C6 | 2.53 | 0.43 |
| 25:YA:270(J):G:H2' | 25:YA:270(K):C:O4' | 2.19 | 0.43 |
| 25:YA:270(V):G:H2' | 25:YA:270(W):G:H8 | 1.83 | 0.43 |
| 25:YA:2712:U:O2' | 25:YA:2712(A):A:H8 | 2.00 | 0.43 |
| 25:YA:2839:G:H5' | 37:YR:46:GLY:HA2 | 1.99 | 0.43 |
| 25:YA:637:A:H4' | 25:YA:638:G:O5' | 2.17 | 0.43 |
| 27:YD:213:ARG:HD2 | 27:YD:217:ARG:O | 2.17 | 0.43 |
| 27:YD:31:LYS:HG3 | 27:YD:32:SER:N | 2.33 | 0.43 |
| 28:YE:101:ARG:NH1 | 28:YE:171:GLU:HB2 | 2.33 | 0.43 |
| 34:YO:22:ILE:HG12 | 34:YO:41:ALA:HA | 1.99 | 0.43 |
| 44:YY:14:LEU:HB2 | 44:YY:75:ILE:HD11 | 1.99 | 0.43 |
| 1:QA:1129:C:H5' | 1:QA:1130:A:H5' | 2.00 | 0.43 |
| 1:QA:477:G:H2' | 1:QA:478:A:H8 | 1.84 | 0.43 |
| 1:QA:925:G:C2 | 1:QA:927:G:C8 | 3.06 | 0.43 |
| 9:QI:89:ASN:HB2 | 9:QI:92:TYR:CE2 | 2.54 | 0.43 |
| 9:QI:114:TYR:HE2 | 10:QJ:59:SER:HA | 1.83 | 0.43 |
| 25:RA:1184:G:OP1 | 49:R3:29:ARG:NH1 | 2.51 | 0.43 |
| 25:RA:1290:C:H2' | 25:RA:1291:C:C6 | 2.52 | 0.43 |
| 25:RA:2052:G:H4' | 28:RE:143:ASN:O | 2.19 | 0.43 |
| 25:RA:2692:C:H2' | 25:RA:2693:A:C8 | 2.52 | 0.43 |
| 25:RA:2693:A:H2' | 25:RA:2694:G:C8 | 2.53 | 0.43 |
| 25:RA:2789:C:H1' | 25:RA:2892:A:H2 | 1.83 | 0.43 |
| 25:RA:2846:G:H2' | 25:RA:2847:U:C6 | 2.53 | 0.43 |
| 25:RA:301:G:C6 | 25:RA:317:G:C6 | 3.07 | 0.43 |
| 25:RA:902:C:H2' | 25:RA:903:C:H6 | 1.82 | 0.43 |
| 28:RE:16:ARG:HG3 | 28:RE:16:ARG:O | 2.18 | 0.43 |
| 29:RF:34:TRP:CD2 | 35:RP:8:PRO:HB3 | 2.54 | 0.43 |
| 25:RA:1257:C:H4' | 29:RF:83:PHE:CE1 | 2.53 | 0.43 |
| 32:RI:99:GLU:OE2 | 32:RI:103:ARG:NH2 | 2.50 | 0.43 |
| 41:RV:55:ALA:HA | 41:RV:101:GLY:HA2 | 2.00 | 0.43 |
| 42:RW:71:VAL:HA | 42:RW:107:LEU:HD23 | 2.00 | 0.43 |
| 1:XA:1301:U:O2' | 1:XA:1302:U:OP1 | 2.32 | 0.43 |
| 1:XA:610:G:C4 | 1:XA:611:A:C8 | 3.06 | 0.43 |
| 1:XA:950:U:H2' | 1:XA:951:G:C8 | 2.53 | 0.43 |
| 1:XA:997:U:H2' | 1:XA:998:G:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:XC:150:LYS:HB3 | 3:XC:201:TYR:HB2 | 2.00 | 0.43 |
| 4:XD:154:ASN:OD1 | 4:XD:155:LEU:N | 2.44 | 0.43 |
| 6:XF:95:GLU:O | 18:XR:32:ARG:NH1 | 2.51 | 0.43 |
| 19:XS:10:PHE:HB2 | 19:XS:39:THR:HB | 2.00 | 0.43 |
| 22:XV:24:C:H2' | 22:XV:25:U:H6 | 1.84 | 0.43 |
| 48:Y2:16:LEU:CD2 | 48:Y2:20:GLU:HG3 | 2.49 | 0.43 |
| 54:Y8:54:GLU:O | 54:Y8:58:ILE:HG12 | 2.18 | 0.43 |
| 55:Y9:9:ARG:CZ | 55:Y9:16:VAL:HB | 2.48 | 0.43 |
| 25:YA:1257:C:H4' | 29:YF:83:PHE:CD1 | 2.53 | 0.43 |
| 25:YA:2183:C:H2' | 25:YA:2184:G:H8 | 1.83 | 0.43 |
| 25:YA:2298:A:H62 | 25:YA:2318:G:H8 | 1.67 | 0.43 |
| 25:YA:2339:G:H2' | 25:YA:2340:G:H8 | 1.83 | 0.43 |
| 25:YA:2475:C:H42 | 25:YA:2529:G:H22 | 1.66 | 0.43 |
| 25:YA:2593:U:H2' | 25:YA:2594:C:C6 | 2.53 | 0.43 |
| 25:YA:2599:G:C8 | 27:YD:236:GLY:HA2 | 2.51 | 0.43 |
| 25:YA:398:G:H2' | 25:YA:399:G:C8 | 2.52 | 0.43 |
| 25:YA:99:U:H4' | 25:YA:101:G:H5' | 2.01 | 0.43 |
| 29:YF:110:LEU:HA | 29:YF:183:VAL:HG12 | 2.00 | 0.43 |
| 29:YF:167:ALA:HA | 29:YF:170:LEU:HD13 | 2.00 | 0.43 |
| 30:YG:144:ILE:HG22 | 30:YG:146:TYR:H | 1.84 | 0.43 |
| 35:YP:85:LEU:HD13 | 35:YP:120:ALA:HB2 | 2.01 | 0.43 |
| 36:YQ:66:ILE:HG13 | 36:YQ:67:ARG:N | 2.33 | 0.43 |
| 1:QA:1032(A):G:H2' | 1:QA:1032(B):G:C8 | 2.53 | 0.43 |
| 1:QA:340:U:H2' | 1:QA:341:C:C6 | 2.54 | 0.43 |
| 1:QA:359:U:H2' | 1:QA:360:A:C8 | 2.53 | 0.43 |
| 1:QA:485:G:HO2' | 1:QA:486:U:H6 | 1.63 | 0.43 |
| 1:QA:718:G:H21 | 18:QR:49:LYS:HE3 | 1.82 | 0.43 |
| 1:QA:574:A:N3 | 1:QA:883:C:H1' | 2.33 | 0.43 |
| 3:QC:88:ARG:NH1 | 3:QC:101:LEU:H | 2.17 | 0.43 |
| 4:QD:63:LYS:O | 4:QD:67:ILE:HG13 | 2.18 | 0.43 |
| 17:QQ:26:GLN:HB3 | 17:QQ:37:LYS:HG2 | 2.01 | 0.43 |
| 22:QW:10:G:H2' | 22:QW:11:A:H8 | 1.83 | 0.43 |
| 25:RA:2271:G:OP1 | 46:R0:18:ALA:HB1 | 2.18 | 0.43 |
| 25:RA:71:A:N6 | 25:RA:114:U:H1' | 2.31 | 0.43 |
| 25:RA:2041:U:H2' | 25:RA:2042:A:H8 | 1.82 | 0.43 |
| 25:RA:2712:U:OP1 | 25:RA:2714:G:H4' | 2.18 | 0.43 |
| 25:RA:18:C:O2' | 25:RA:553:U:OP1 | 2.37 | 0.43 |
| 25:RA:689:A:H2' | 25:RA:690:G:H8 | 1.84 | 0.43 |
| 28:RE:134:ILE:HA | 28:RE:137:HIS:ND1 | 2.34 | 0.43 |
| 13:QM:3:ARG:NH2 | 30:RG:113:ARG:HH21 | 2.14 | 0.43 |
| 36:RQ:17:LEU:HD11 | 36:RQ:41:TRP:NE1 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1000:A:H2' | 1:XA:1001:G:C8 | 2.53 | 0.43 |
| 1:XA:1454:G:H2' | 1:XA:1455:G:H8 | 1.83 | 0.43 |
| 1:XA:41:G:H2' | 1:XA:42:G:H8 | 1.83 | 0.43 |
| 1:XA:923:A:H2' | 1:XA:924:C:C6 | 2.54 | 0.43 |
| 4:XD:190:ASP:OD1 | 4:XD:191:ARG:N | 2.45 | 0.43 |
| 1:XA:363:A:OP1 | 12:XL:33:ARG:HD3 | 2.18 | 0.43 |
| 13:XM:96:LEU:HB3 | 13:XM:97:PRO:HD2 | 2.00 | 0.43 |
| 1:XA:674:G:H1' | 18:XR:81:PHE:CE2 | 2.54 | 0.43 |
| 20:XT:54:LYS:HG3 | 20:XT:57:ARG:NH2 | 2.33 | 0.43 |
| 22:XV:15:G:H22 | 22:XV:49:C:H41 | 1.66 | 0.43 |
| 24:XY:39:U:H2' | 24:XY:40:C:H6 | 1.82 | 0.43 |
| 53:Y7:17:GLY:O | 53:Y7:21:ARG:HG2 | 2.19 | 0.43 |
| 25:YA:1930:G:H2' | 25:YA:1968:G:H1 | 1.83 | 0.43 |
| 25:YA:2099:U:H2' | 25:YA:2100:G:C8 | 2.53 | 0.43 |
| 25:YA:608:A:H2' | 25:YA:609:A:C8 | 2.53 | 0.43 |
| 28:YE:56:PRO:HD2 | 28:YE:58:ARG:NH2 | 2.32 | 0.43 |
| 31:YH:46:GLU:HB2 | 31:YH:49:VAL:HG23 | 1.99 | 0.43 |
| 40:YU:87:GLY:O | 41:YV:50:PRO:HD3 | 2.19 | 0.43 |
| 1:QA:1135:U:H4' | 1:QA:1136:U:H5 | 1.84 | 0.43 |
| 3:QC:19:GLU:O | 3:QC:40:ARG:NH2 | 2.51 | 0.43 |
| 1:QA:1151:A:O2' | 10:QJ:70:ARG:NH2 | 2.52 | 0.43 |
| 11:QK:48:ILE:HD11 | 11:QK:64:ALA:HA | 2.00 | 0.43 |
| 12:QL:103:GLY:N | 12:QL:107:ALA:O | 2.42 | 0.43 |
| 22:QV:75:C:O2' | 22:QV:76:C:H5' | 2.18 | 0.43 |
| 25:RA:669:G:N3 | 25:RA:669:G:H2' | 2.33 | 0.43 |
| 25:RA:679:C:H2' | 25:RA:680:G:C8 | 2.54 | 0.43 |
| 27:RD:44:ASN:HB3 | 27:RD:49:ILE:HA | 1.99 | 0.43 |
| 29:RF:9:ILE:HG12 | 29:RF:123:LEU:HD23 | 2.01 | 0.43 |
| 30:RG:111:LEU:HB3 | 30:RG:117:PHE:CZ | 2.53 | 0.43 |
| 28:RE:152:LYS:HG3 | 33:RN:78:TYR:CE1 | 2.53 | 0.43 |
| 44:RY:8:LYS:HD3 | 44:RY:97:ARG:HH21 | 1.82 | 0.43 |
| 1:XA:1129:C:H4' | 1:XA:1130:A:H8 | 1.84 | 0.43 |
| 1:XA:1129:C:N4 | 1:XA:1133:G:O6 | 2.51 | 0.43 |
| 1:XA:1488:G:H2' | 1:XA:1489:G:H8 | 1.83 | 0.43 |
| 2:XB:74:LYS:NZ | 2:XB:206:ASP:OD1 | 2.28 | 0.43 |
| 3:XC:52:LEU:H | 3:XC:52:LEU:HD23 | 1.83 | 0.43 |
| 4:XD:100:ARG:NH2 | 4:XD:136:PRO:O | 2.52 | 0.43 |
| 7:XG:46:ALA:O | 7:XG:50:ILE:HG12 | 2.18 | 0.43 |
| 1:XA:1226:C:O2' | 13:XM:111:LYS:NZ | 2.48 | 0.43 |
| 6:XF:97:PHE:CD2 | 18:XR:31:LEU:HD21 | 2.53 | 0.43 |
| 25:YA:1438:U:H2' | 25:YA:1439:A:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1458:C:H4' | 25:YA:1459:G:O4' | 2.18 | 0.43 |
| 25:YA:1509:C:H2' | 25:YA:1511:A:C8 | 2.53 | 0.43 |
| 25:YA:1683:C:H2' | 25:YA:1684:C:C6 | 2.54 | 0.43 |
| 25:YA:1770:G:H2' | 25:YA:1771:C:C6 | 2.53 | 0.43 |
| 25:YA:2684:U:H5'' | 39:YT:75:ILE:HD13 | 1.99 | 0.43 |
| 25:YA:196:A:N7 | 25:YA:805:G:C5 | 2.87 | 0.43 |
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:CD2 | 2.53 | 0.43 |
| 27:YD:11:PRO:O | 27:YD:12:SER:OG | 2.32 | 0.43 |
| 25:YA:1788:C:H5'' | 27:YD:225:ALA:HB1 | 2.00 | 0.43 |
| 30:YG:169:ALA:O | 30:YG:173:LEU:HG | 2.18 | 0.43 |
| 25:YA:2746:U:H5'' | 31:YH:138:LYS:HE2 | 1.99 | 0.43 |
| 25:YA:831:G:O2' | 35:YP:38:GLN:OE1 | 2.34 | 0.43 |
| 25:YA:244:A:H4' | 35:YP:74:GLU:HB2 | 1.99 | 0.43 |
| 25:YA:296:C:O3' | 44:YY:95:LYS:NZ | 2.51 | 0.43 |
| 45:YZ:102:LEU:HD21 | 45:YZ:124:ILE:HD12 | 2.00 | 0.43 |
| 1:QA:109:A:C6 | 1:QA:326:G:C6 | 3.07 | 0.43 |
| 1:QA:1014:A:C2 | 1:QA:1219:U:H1' | 2.54 | 0.43 |
| 1:QA:923:A:H2' | 1:QA:924:C:C6 | 2.53 | 0.43 |
| 1:QA:963:G:H21 | 10:QJ:55:LYS:HE2 | 1.83 | 0.43 |
| 2:QB:167:PRO:HG3 | 2:QB:188:ALA:HB2 | 1.99 | 0.43 |
| 5:QE:48:ALA:HB2 | 5:QE:57:LYS:HE3 | 1.99 | 0.43 |
| 7:QG:143:ARG:HD3 | 22:QW:42:C:O3' | 2.19 | 0.43 |
| 1:QA:134:A:H61 | 16:QP:25:ARG:HH12 | 1.67 | 0.43 |
| 25:RA:1042:G:H2' | 25:RA:1043:C:C6 | 2.53 | 0.43 |
| 25:RA:1116:C:H2' | 25:RA:1117:G:H8 | 1.84 | 0.43 |
| 25:RA:2469:A:H5'' | 25:RA:2470:G:H8 | 1.82 | 0.43 |
| 25:RA:910:A:N3 | 25:RA:2264:C:O2' | 2.45 | 0.43 |
| 27:RD:69:ARG:NH1 | 27:RD:105:ILE:HG12 | 2.34 | 0.43 |
| 30:RG:112:PRO:HB3 | 50:R4:40:HIS:CD2 | 2.53 | 0.43 |
| 13:QM:7:VAL:HB | 30:RG:115:ARG:HH12 | 1.82 | 0.43 |
| 30:RG:144:ILE:HG22 | 30:RG:146:TYR:H | 1.84 | 0.43 |
| 32:RI:82:ARG:HA | 32:RI:145:VAL:HG12 | 2.01 | 0.43 |
| 34:RO:93:PRO:HB3 | 34:RO:114:ILE:HD11 | 2.00 | 0.43 |
| 25:RA:863:A:OP1 | 36:RQ:21:THR:HB | 2.19 | 0.43 |
| 36:RQ:24:GLY:H | 36:RQ:101:ARG:CD | 2.29 | 0.43 |
| 39:RT:57:PHE:CG | 39:RT:58:ASN:N | 2.87 | 0.43 |
| 40:RU:91:ASP:C | 40:RU:93:LYS:N | 2.72 | 0.43 |
| 44:RY:28:LYS:N | 44:RY:38:ILE:O | 2.50 | 0.43 |
| 1:XA:105:G:H2' | 1:XA:106:C:H6 | 1.83 | 0.43 |
| 1:XA:1167:A:H2' | 1:XA:1169:A:C8 | 2.53 | 0.43 |
| 1:XA:1355:G:H2' | 1:XA:1356:G:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:281:G:OP2 | 1:XA:281:G:H8 | 2.01 | 0.43 |
| 1:XA:373:A:C2 | 1:XA:374:A:C8 | 3.06 | 0.43 |
| 1:XA:825:G:H2' | 1:XA:826:C:C6 | 2.54 | 0.43 |
| 8:XH:103:VAL:HG12 | 8:XH:108:GLY:HA3 | 2.00 | 0.43 |
| 1:XA:539:A:OP2 | 12:XL:115:LYS:HD3 | 2.18 | 0.43 |
| 17:XQ:28:PRO:HG3 | 17:XQ:35:VAL:HG22 | 2.01 | 0.43 |
| 46:Y0:72:ARG:HB3 | 46:Y0:75:LEU:HB2 | 2.01 | 0.43 |
| 47:Y1:44:PRO:HG2 | 47:Y1:46:LEU:CD1 | 2.48 | 0.43 |
| 25:YA:2742:C:C4 | 55:Y9:33:LYS:NZ | 2.85 | 0.43 |
| 25:YA:1869:G:H5' | 25:YA:1870:C:OP2 | 2.19 | 0.43 |
| 25:YA:191:A:H2' | 25:YA:192:C:C6 | 2.53 | 0.43 |
| 25:YA:2176:A:H2' | 25:YA:2177:C:C6 | 2.54 | 0.43 |
| 25:YA:2521:C:H2' | 25:YA:2522:U:C6 | 2.54 | 0.43 |
| 25:YA:2554:U:H2' | 25:YA:2555:U:C6 | 2.53 | 0.43 |
| 25:YA:2577:A:H5' | 51:Y5:3:LYS:HZ2 | 1.83 | 0.43 |
| 25:YA:2649:U:H2' | 25:YA:2650:U:H6 | 1.83 | 0.43 |
| 25:YA:270(E):G:H2' | 25:YA:270(F):U:C6 | 2.53 | 0.43 |
| 25:YA:554:U:H2' | 25:YA:556:G:H8 | 1.84 | 0.43 |
| 25:YA:609(A):G:H2' | 25:YA:610:C:C6 | 2.54 | 0.43 |
| 27:YD:133:LEU:HG | 27:YD:189:CYS:O | 2.19 | 0.43 |
| 25:YA:442:G:H1' | 29:YF:48:THR:HG21 | 2.00 | 0.43 |
| 42:YW:82:LEU:HD23 | 42:YW:84:ARG:NH2 | 2.33 | 0.43 |
| 43:YX:26:TYR:CD2 | 43:YX:89:ILE:HD12 | 2.47 | 0.43 |
| 1:QA:1254:C:OP1 | 10:QJ:45:ARG:NE | 2.29 | 0.43 |
| 1:QA:361:G:H2' | 1:QA:362:G:O4' | 2.19 | 0.43 |
| 5:QE:5:ASP:OD1 | 5:QE:6:PHE:N | 2.52 | 0.43 |
| 12:QL:24:VAL:HG13 | 12:QL:98:TYR:CE1 | 2.54 | 0.43 |
| 13:QM:14:ARG:NH2 | 13:QM:16:ASP:OD2 | 2.51 | 0.43 |
| 25:RA:116:C:H2' | 25:RA:117:G:O4' | 2.19 | 0.43 |
| 25:RA:1914:C:H2' | 25:RA:1915:U:O4' | 2.18 | 0.43 |
| 25:RA:2168:G:N3 | 25:RA:2168:G:H2' | 2.34 | 0.43 |
| 25:RA:2243:U:H2' | 25:RA:2244:U:H6 | 1.82 | 0.43 |
| 25:RA:2329:G:H2' | 25:RA:2330:G:C8 | 2.54 | 0.43 |
| 25:RA:2443:C:H2' | 25:RA:2444:G:C8 | 2.54 | 0.43 |
| 25:RA:2022:U:O2' | 25:RA:2617:C:H5' | 2.19 | 0.43 |
| 25:RA:2663:G:H2' | 25:RA:2664:G:O4' | 2.19 | 0.43 |
| 25:RA:1662:C:O2' | 25:RA:2687:U:OP1 | 2.37 | 0.43 |
| 25:RA:507:A:H5'' | 25:RA:508:G:H5' | 2.01 | 0.43 |
| 25:RA:687:C:H5'' | 53:R7:2:LYS:HE2 | 2.00 | 0.43 |
| 33:RN:13:TRP:HB2 | 33:RN:133:GLN:HB3 | 2.00 | 0.43 |
| 38:RS:42:ASP:C | 38:RS:44:LYS:H | 2.21 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:XH:12:ARG:HD2 | 8:XH:26:VAL:HG12 | 2.00 | 0.43 |
| 9:XI:48:GLU:N | 9:XI:49:PRO:HD2 | 2.34 | 0.43 |
| 25:YA:2742:C:O2' | 55:Y9:32:HIS:O | 2.25 | 0.43 |
| 25:YA:1605:C:H2' | 25:YA:1606:G:O4' | 2.19 | 0.43 |
| 25:YA:2241:A:H2' | 25:YA:2242:G:H8 | 1.81 | 0.43 |
| 25:YA:2319:G:O6 | 38:YS:4:LEU:HB2 | 2.19 | 0.43 |
| 25:YA:273:G:H1 | 25:YA:364:C:H42 | 1.65 | 0.43 |
| 25:YA:767:U:H2' | 25:YA:768:G:H8 | 1.84 | 0.43 |
| 25:YA:816:C:H2' | 25:YA:817:C:C6 | 2.54 | 0.43 |
| 29:YF:155:LEU:HD23 | 29:YF:186:ILE:HD13 | 2.01 | 0.43 |
| 30:YG:11:TYR:HD1 | 30:YG:176:LEU:HD21 | 1.83 | 0.43 |
| 32:YI:5:LEU:HD21 | 32:YI:12:LEU:HB3 | 2.00 | 0.43 |
| 1:QA:1103:C:H2' | 1:QA:1104:G:O4' | 2.19 | 0.43 |
| 1:QA:1128:C:OP1 | 9:QI:66:ARG:NH2 | 2.52 | 0.43 |
| 1:QA:1410:G:H2' | 1:QA:1411:C:C6 | 2.54 | 0.43 |
| 1:QA:381:C:H2' | 1:QA:382:A:O4' | 2.19 | 0.43 |
| 1:QA:701:C:H1' | 1:QA:703:G:C2 | 2.54 | 0.43 |
| 1:QA:797:C:OP1 | 11:QK:124:LYS:HD3 | 2.19 | 0.43 |
| 13:QM:53:VAL:HG12 | 13:QM:57:ARG:NE | 2.33 | 0.43 |
| 47:R1:40:ARG:HH12 | 47:R1:42:GLN:HG2 | 1.84 | 0.43 |
| 25:RA:1204:A:O2' | 25:RA:1205:U:O5' | 2.36 | 0.43 |
| 25:RA:2455:G:H2' | 25:RA:2456:C:H6 | 1.84 | 0.43 |
| 25:RA:2593:U:H2' | 25:RA:2594:C:C6 | 2.53 | 0.43 |
| 25:RA:2637:U:H5'' | 28:RE:82:ARG:HH12 | 1.84 | 0.43 |
| 25:RA:605:C:O2 | 25:RA:657:U:O2' | 2.37 | 0.43 |
| 26:RB:88:C:H2' | 26:RB:89:G:C8 | 2.54 | 0.43 |
| 36:RQ:65:PHE:O | 36:RQ:67:ARG:HG3 | 2.19 | 0.43 |
| 36:RQ:79:LEU:O | 36:RQ:79:LEU:HD23 | 2.19 | 0.43 |
| 37:RR:38:VAL:HB | 37:RR:39:PRO:HD3 | 2.00 | 0.43 |
| 1:XA:1067:A:N1 | 1:XA:1108:G:O2' | 2.49 | 0.43 |
| 1:XA:1225:A:N3 | 1:XA:1225:A:H2' | 2.34 | 0.43 |
| 1:XA:1250:A:H2' | 1:XA:1251:A:C8 | 2.53 | 0.43 |
| 1:XA:1330:U:H5'' | 1:XA:1331:G:OP2 | 2.19 | 0.43 |
| 1:XA:1389:C:H2' | 1:XA:1390:U:C6 | 2.54 | 0.43 |
| 1:XA:711:G:H2' | 1:XA:712:A:H8 | 1.84 | 0.43 |
| 1:XA:93:U:H2' | 1:XA:95:G:O4' | 2.19 | 0.43 |
| 2:XB:160:ASP:O | 2:XB:183:PRO:HD2 | 2.18 | 0.43 |
| 3:XC:157:ILE:HD13 | 3:XC:166:GLU:HG2 | 2.01 | 0.43 |
| 6:XF:8:ILE:HD13 | 6:XF:26:ILE:HD13 | 2.01 | 0.43 |
| 7:XG:147:ALA:CB | 22:XW:42:C:H5' | 2.49 | 0.43 |
| 11:XK:67:ASP:OD1 | 11:XK:71:LYS:HE3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 15:XO:21:ASP:OD2 | 15:XO:24:SER:HB2 | 2.18 | 0.43 |
| 18:XR:70:ILE:O | 18:XR:74:ARG:HB2 | 2.19 | 0.43 |
| 25:YA:2433:A:H1' | 47:Y1:21:ARG:HH22 | 1.84 | 0.43 |
| 55:Y9:25:VAL:HG23 | 55:Y9:34:GLN:N | 2.33 | 0.43 |
| 25:YA:1637:A:H4' | 25:YA:2711:A:O2' | 2.19 | 0.43 |
| 25:YA:1825:A:H2' | 25:YA:1826:G:C8 | 2.54 | 0.43 |
| 25:YA:1842:G:H2' | 25:YA:1843:C:H6 | 1.84 | 0.43 |
| 25:YA:1878:G:H2' | 25:YA:1879:C:C6 | 2.53 | 0.43 |
| 25:YA:1918:A:O2' | 25:YA:1920:C:N4 | 2.52 | 0.43 |
| 25:YA:2064:C:H2' | 25:YA:2065:C:H6 | 1.83 | 0.43 |
| 25:YA:375:C:H2' | 25:YA:376:C:C6 | 2.53 | 0.43 |
| 25:YA:664:C:H2' | 25:YA:665:C:H6 | 1.84 | 0.43 |
| 25:YA:709:U:H2' | 25:YA:710:G:H8 | 1.84 | 0.43 |
| 25:YA:729:G:H5' | 25:YA:730:C:H5'' | 2.00 | 0.43 |
| 25:YA:860:U:OP2 | 25:YA:916:G:N1 | 2.50 | 0.43 |
| 36:YQ:23:GLY:HA3 | 36:YQ:101:ARG:HD3 | 2.00 | 0.43 |
| 36:YQ:65:PHE:O | 36:YQ:67:ARG:HG3 | 2.19 | 0.43 |
| 45:YZ:4:ARG:HA | 45:YZ:59:LEU:H | 1.83 | 0.43 |
| 45:YZ:59:LEU:O | 45:YZ:60:GLU:HG2 | 2.18 | 0.43 |
| 1:QA:148:G:H2' | 1:QA:149:A:H8 | 1.84 | 0.43 |
| 1:QA:323:U:H2' | 1:QA:324:G:O4' | 2.18 | 0.43 |
| 7:QG:66:VAL:O | 7:QG:70:LYS:HG3 | 2.19 | 0.43 |
| 8:QH:103:VAL:HG12 | 8:QH:108:GLY:HA3 | 2.01 | 0.43 |
| 9:QI:28:VAL:HG22 | 9:QI:63:ILE:HB | 2.01 | 0.43 |
| 12:QL:104:VAL:HG12 | 12:QL:105:TYR:N | 2.26 | 0.43 |
| 25:RA:111:A:H5' | 48:R2:69:ARG:HH11 | 1.83 | 0.43 |
| 53:R7:26:GLY:O | 53:R7:30:VAL:HG23 | 2.19 | 0.43 |
| 25:RA:1105:U:H2' | 25:RA:1106:G:C8 | 2.51 | 0.43 |
| 25:RA:1660:C:H5' | 25:RA:2712(A):A:H61 | 1.83 | 0.43 |
| 25:RA:2291:U:H2' | 25:RA:2292:C:C6 | 2.54 | 0.43 |
| 25:RA:2514:U:H2' | 25:RA:2515:C:C6 | 2.54 | 0.43 |
| 25:RA:2784:C:H2' | 25:RA:2785:C:H6 | 1.83 | 0.43 |
| 25:RA:638:G:C5 | 25:RA:651:G:C2 | 3.06 | 0.43 |
| 25:RA:828:U:H4' | 25:RA:831:G:N1 | 2.33 | 0.43 |
| 28:RE:38:THR:HG23 | 28:RE:41:LYS:H | 1.83 | 0.43 |
| 28:RE:52:LEU:HB2 | 28:RE:75:VAL:HB | 2.00 | 0.43 |
| 29:RF:64:ILE:HG23 | 29:RF:65:TRP:H | 1.84 | 0.43 |
| 25:RA:2198:A:C2 | 32:RI:29:TYR:HB2 | 2.54 | 0.43 |
| 44:RY:39:VAL:HB | 44:RY:42:VAL:HB | 2.01 | 0.43 |
| 1:XA:1169:A:H2' | 1:XA:1170:A:C8 | 2.53 | 0.43 |
| 1:XA:1226:C:H2' | 13:XM:103:THR:HB | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1241:G:H2' | 1:XA:1242:C:H6 | 1.84 | 0.43 |
| 1:XA:1391:U:H2' | 1:XA:1392:G:C8 | 2.53 | 0.43 |
| 1:XA:1446:A:O2' | 1:XA:1447:G:O4' | 2.36 | 0.43 |
| 1:XA:253:U:H2' | 1:XA:254:G:H8 | 1.84 | 0.43 |
| 1:XA:376:G:H1 | 1:XA:387:U:H3 | 1.65 | 0.43 |
| 1:XA:381:C:H2' | 1:XA:382:A:O4' | 2.19 | 0.43 |
| 19:XS:22:LEU:O | 19:XS:26:GLY:HA2 | 2.18 | 0.43 |
| 54:Y8:29:LYS:HG3 | 54:Y8:30:ARG:N | 2.27 | 0.43 |
| 25:YA:2741:A:H5'' | 55:Y9:31:LYS:HA | 2.00 | 0.43 |
| 25:YA:1425:G:H2' | 25:YA:1426:G:C8 | 2.54 | 0.43 |
| 25:YA:1679:U:H1' | 25:YA:1989:G:H21 | 1.84 | 0.43 |
| 25:YA:2086:U:H2' | 25:YA:2087:G:C8 | 2.53 | 0.43 |
| 25:YA:2697:G:H2' | 25:YA:2698:U:C6 | 2.54 | 0.43 |
| 25:YA:605:C:O2 | 25:YA:657:U:O2' | 2.37 | 0.43 |
| 27:YD:44:ASN:HB2 | 27:YD:48:ARG:O | 2.18 | 0.43 |
| 27:YD:72:LYS:HG3 | 27:YD:97:TYR:CE2 | 2.54 | 0.43 |
| 29:YF:178:PRO:HG2 | 29:YF:179:GLU:OE1 | 2.19 | 0.43 |
| 38:YS:42:ASP:C | 38:YS:44:LYS:H | 2.23 | 0.43 |
| 1:QA:1000:A:H2' | 1:QA:1001:G:C8 | 2.54 | 0.42 |
| 1:QA:1104:G:O2' | 2:QB:111:ARG:NH1 | 2.53 | 0.42 |
| 1:QA:1370:G:H2' | 1:QA:1371:G:H8 | 1.84 | 0.42 |
| 1:QA:434:U:H2' | 1:QA:435:C:C6 | 2.54 | 0.42 |
| 1:QA:742:G:OP2 | 15:QO:35:ARG:NH2 | 2.52 | 0.42 |
| 1:QA:892:A:H2' | 1:QA:893:C:H6 | 1.83 | 0.42 |
| 7:QG:13:GLN:O | 7:QG:24:THR:HG21 | 2.19 | 0.42 |
| 1:QA:1147:C:O2 | 9:QI:16:ARG:NH2 | 2.52 | 0.42 |
| 1:QA:963:G:N3 | 10:QJ:55:LYS:HE2 | 2.34 | 0.42 |
| 25:RA:1032:A:HO2' | 25:RA:1033:U:P | 2.42 | 0.42 |
| 25:RA:1946:U:H2' | 25:RA:1947:C:C6 | 2.54 | 0.42 |
| 25:RA:2073:C:H5'' | 27:RD:229:VAL:HG22 | 2.01 | 0.42 |
| 25:RA:2216:G:H2' | 25:RA:2217:G:H8 | 1.84 | 0.42 |
| 25:RA:2579:C:O2' | 28:RE:131:ALA:HA | 2.18 | 0.42 |
| 25:RA:910:A:C6 | 36:RQ:13:GLN:HG3 | 2.54 | 0.42 |
| 27:RD:77:ALA:HB2 | 27:RD:97:TYR:CD1 | 2.54 | 0.42 |
| 28:RE:82:ARG:O | 28:RE:83:ASP:HB2 | 2.19 | 0.42 |
| 29:RF:184:TYR:O | 29:RF:188:ARG:HG3 | 2.19 | 0.42 |
| 25:RA:2310:A:N6 | 30:RG:79:ASN:OD1 | 2.52 | 0.42 |
| 1:XA:1290:G:N3 | 1:XA:1290:G:H2' | 2.33 | 0.42 |
| 3:XC:56:ASP:HB2 | 3:XC:67:THR:HB | 2.01 | 0.42 |
| 3:XC:68:VAL:HG12 | 3:XC:70:VAL:HG23 | 1.99 | 0.42 |
| 19:XS:3:ARG:HH22 | 19:XS:11:VAL:HG11 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:Y6:38:LYS:HB2 | 52:Y6:49:HIS:CE1 | 2.54 | 0.42 |
| 25:YA:1429:G:H2' | 25:YA:1430:C:H6 | 1.84 | 0.42 |
| 25:YA:2525:G:O2' | 25:YA:2526:G:C8 | 2.69 | 0.42 |
| 25:YA:2679:A:OP2 | 28:YE:160:TYR:OH | 2.36 | 0.42 |
| 25:YA:270(R):G:H2' | 25:YA:270(S):G:C8 | 2.54 | 0.42 |
| 25:YA:2740:A:C6 | 25:YA:2764:A:C5 | 3.07 | 0.42 |
| 25:YA:532:A:N1 | 25:YA:2019:A:H2 | 2.17 | 0.42 |
| 25:YA:648:G:H2' | 25:YA:649:G:H8 | 1.84 | 0.42 |
| 31:YH:9:ILE:HA | 31:YH:10:PRO:HD3 | 1.88 | 0.42 |
| 42:YW:11:ARG:HH21 | 42:YW:98:LYS:HD3 | 1.83 | 0.42 |
| 1:QA:1250:A:H2' | 1:QA:1251:A:C8 | 2.54 | 0.42 |
| 1:QA:336:C:H1' | 1:QA:1468:A:H2 | 1.84 | 0.42 |
| 1:QA:621:A:H2' | 1:QA:622:A:H8 | 1.84 | 0.42 |
| 4:QD:60:GLU:OE2 | 4:QD:198:VAL:HA | 2.19 | 0.42 |
| 7:QG:152:ALA:O | 7:QG:155:ARG:HG3 | 2.19 | 0.42 |
| 18:QR:70:ILE:O | 18:QR:74:ARG:HB2 | 2.19 | 0.42 |
| 11:QK:54:ARG:NH1 | 22:QW:40:C:H4' | 2.33 | 0.42 |
| 25:RA:857:C:OP1 | 46:R0:69:PHE:HD2 | 2.02 | 0.42 |
| 25:RA:1212:G:O2' | 25:RA:1213:A:OP2 | 2.35 | 0.42 |
| 25:RA:1234:U:H2' | 25:RA:1235:G:O4' | 2.18 | 0.42 |
| 25:RA:1412:A:H2' | 25:RA:1413:G:C8 | 2.54 | 0.42 |
| 25:RA:1509:C:N3 | 25:RA:1511:A:N6 | 2.67 | 0.42 |
| 25:RA:2403:C:N3 | 25:RA:2415:G:N1 | 2.67 | 0.42 |
| 25:RA:2528:U:H2' | 25:RA:2530:A:O5' | 2.19 | 0.42 |
| 25:RA:962:G:H2' | 25:RA:963:U:C6 | 2.53 | 0.42 |
| 27:RD:175:LEU:HD12 | 27:RD:185:VAL:HG21 | 2.00 | 0.42 |
| 27:RD:52:ARG:NH1 | 27:RD:249:PRO:HG2 | 2.34 | 0.42 |
| 30:RG:82:LEU:HD21 | 30:RG:88:ILE:HG21 | 2.00 | 0.42 |
| 31:RH:55:PRO:HG2 | 31:RH:61:HIS:CE1 | 2.54 | 0.42 |
| 36:RQ:48:GLU:OE2 | 36:RQ:51:ARG:NH2 | 2.52 | 0.42 |
| 39:RT:20:PRO:HD2 | 39:RT:86:ILE:HG23 | 2.00 | 0.42 |
| 1:XA:1000:A:H2' | 1:XA:1001:G:H8 | 1.84 | 0.42 |
| 1:XA:1154:G:H2' | 1:XA:1155:G:H8 | 1.85 | 0.42 |
| 1:XA:1348:U:N3 | 1:XA:1374:A:H2 | 2.12 | 0.42 |
| 1:XA:824:C:H2' | 1:XA:825:G:H8 | 1.83 | 0.42 |
| 1:XA:895:G:H2' | 1:XA:896:C:C6 | 2.54 | 0.42 |
| 1:XA:998(A):C:H2' | 1:XA:999:U:C6 | 2.54 | 0.42 |
| 9:XI:22:GLY:HA3 | 9:XI:60:ASP:OD2 | 2.19 | 0.42 |
| 10:XJ:33:GLN:HB2 | 10:XJ:75:ILE:HD11 | 2.01 | 0.42 |
| 15:XO:17:ARG:HH12 | 15:XO:77:ARG:NH1 | 2.15 | 0.42 |
| 19:XS:41:VAL:H | 19:XS:44:MET:HE3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:1448:G:H5' | 25:YA:1449:A:OP1 | 2.19 | 0.42 |
| 25:YA:1526:G:H2' | 25:YA:1527:G:C8 | 2.54 | 0.42 |
| 25:YA:1528:A:N6 | 25:YA:1545:A:N1 | 2.66 | 0.42 |
| 25:YA:1812:A:C4' | 27:YD:46:GLN:HE22 | 2.32 | 0.42 |
| 25:YA:1825:A:H2' | 25:YA:1826:G:H8 | 1.83 | 0.42 |
| 25:YA:530:G:N1 | 25:YA:2022:U:OP1 | 2.52 | 0.42 |
| 25:YA:2515:C:H2' | 25:YA:2516:G:H8 | 1.83 | 0.42 |
| 25:YA:2641:G:H2' | 25:YA:2642:G:H8 | 1.85 | 0.42 |
| 25:YA:49:A:H5'' | 25:YA:51:G:O4' | 2.19 | 0.42 |
| 25:YA:808:G:H2' | 25:YA:809:G:H8 | 1.84 | 0.42 |
| 25:YA:1130:U:N3 | 28:YE:147:PRO:HB3 | 2.33 | 0.42 |
| 31:YH:152:ARG:C | 31:YH:152:ARG:HD2 | 2.39 | 0.42 |
| 40:YU:17:ILE:HG13 | 40:YU:32:PHE:HE1 | 1.84 | 0.42 |
| 43:YX:11:PRO:HD3 | 48:Y2:37:PHE:CE1 | 2.54 | 0.42 |
| 43:YX:70:LEU:H | 43:YX:70:LEU:HD23 | 1.84 | 0.42 |
| 1:QA:1240:U:OP1 | 7:QG:119:ARG:NH2 | 2.52 | 0.42 |
| 1:QA:219:C:H2' | 1:QA:220:G:O4' | 2.20 | 0.42 |
| 1:QA:424:G:H2' | 1:QA:425:G:C8 | 2.54 | 0.42 |
| 1:QA:45:U:H2' | 1:QA:46:G:H8 | 1.82 | 0.42 |
| 3:QC:91:LEU:HB3 | 3:QC:99:VAL:HG11 | 2.00 | 0.42 |
| 4:QD:119:GLN:HB3 | 4:QD:119:GLN:OE1 | 2.20 | 0.42 |
| 25:RA:103:A:OP2 | 25:RA:103:A:H8 | 2.02 | 0.42 |
| 25:RA:1043:C:H2' | 25:RA:1044:G:O4' | 2.20 | 0.42 |
| 25:RA:1199:U:H2' | 25:RA:1200:C:C6 | 2.54 | 0.42 |
| 25:RA:1423:G:H2' | 25:RA:1424:G:H8 | 1.83 | 0.42 |
| 25:RA:2262:U:H4' | 25:RA:2328:A:C2 | 2.55 | 0.42 |
| 25:RA:2420:C:OP1 | 54:R8:34:TRP:HB3 | 2.19 | 0.42 |
| 25:RA:380:U:H5' | 47:R1:18:ILE:HD12 | 2.02 | 0.42 |
| 25:RA:534:U:H2' | 25:RA:535:C:C6 | 2.55 | 0.42 |
| 25:RA:565:C:H2' | 25:RA:566:U:C6 | 2.54 | 0.42 |
| 25:RA:883:G:H22 | 25:RA:892:G:N2 | 2.15 | 0.42 |
| 25:RA:2619:C:H5'' | 28:RE:152:LYS:HA | 2.01 | 0.42 |
| 28:RE:18:ASP:HB3 | 39:RT:82:LEU:HD11 | 2.02 | 0.42 |
| 36:RQ:30:GLY:CA | 36:RQ:107:ALA:HB2 | 2.49 | 0.42 |
| 25:RA:1651:G:OP2 | 37:RR:40:LYS:NZ | 2.51 | 0.42 |
| 37:RR:26:LYS:HE2 | 37:RR:70:LEU:O | 2.19 | 0.42 |
| 1:XA:1091:U:C2 | 1:XA:1095:U:C4 | 3.07 | 0.42 |
| 1:XA:603:U:H2' | 1:XA:604:G:H8 | 1.85 | 0.42 |
| 1:XA:679:C:H2' | 1:XA:680:C:C6 | 2.54 | 0.42 |
| 1:XA:966:G:N2 | 22:XV:35:C:H5' | 2.34 | 0.42 |
| 3:XC:189:ALA:CB | 3:XC:196:LEU:HB2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:XL:33:ARG:N | 12:XL:85:ILE:HG22 | 2.34 | 0.42 |
| 1:XA:1202:G:O4' | 14:XN:29:ARG:NH1 | 2.53 | 0.42 |
| 25:YA:2526:G:H1' | 55:Y9:28:GLU:OE1 | 2.19 | 0.42 |
| 25:YA:1802:A:H2' | 25:YA:1803:A:C8 | 2.54 | 0.42 |
| 25:YA:1907:G:H2' | 25:YA:1908:C:C6 | 2.54 | 0.42 |
| 25:YA:2008:C:H2' | 25:YA:2009:G:H8 | 1.84 | 0.42 |
| 25:YA:2740:A:C6 | 25:YA:2741:A:N6 | 2.87 | 0.42 |
| 25:YA:2744:G:C6 | 25:YA:2761:G:C5 | 3.07 | 0.42 |
| 25:YA:2747:G:N2 | 25:YA:2757:A:H62 | 2.15 | 0.42 |
| 25:YA:629:G:H1' | 25:YA:639:U:H1' | 2.01 | 0.42 |
| 25:YA:839:U:H1' | 25:YA:1191:G:H1' | 2.00 | 0.42 |
| 25:YA:947:G:H2' | 25:YA:948:G:H8 | 1.84 | 0.42 |
| 27:YD:228:PRO:HD3 | 27:YD:235:GLY:CA | 2.50 | 0.42 |
| 28:YE:171:GLU:HB3 | 28:YE:185:LYS:HD3 | 2.01 | 0.42 |
| 29:YF:73:ALA:HB3 | 29:YF:75:HIS:HE1 | 1.85 | 0.42 |
| 31:YH:12:PRO:HD3 | 31:YH:48:GLY:O | 2.19 | 0.42 |
| 33:YN:22:THR:HG23 | 33:YN:62:VAL:HA | 2.00 | 0.42 |
| 1:QA:1015:A:H2' | 1:QA:1016:A:C8 | 2.53 | 0.42 |
| 1:QA:1022:G:H2' | 1:QA:1023:G:C8 | 2.54 | 0.42 |
| 1:QA:1149:C:H2' | 1:QA:1150:U:C6 | 2.54 | 0.42 |
| 2:QB:166:ASP:HB3 | 2:QB:169:LYS:HB3 | 2.01 | 0.42 |
| 5:QE:51:VAL:HB | 5:QE:52:PRO:HD3 | 2.02 | 0.42 |
| 6:QF:47:ARG:NH2 | 6:QF:57:GLN:OE1 | 2.53 | 0.42 |
| 22:QW:23:G:C2 | 22:QW:24:C:C5 | 3.07 | 0.42 |
| 25:RA:2041:U:H2' | 25:RA:2042:A:C8 | 2.55 | 0.42 |
| 25:RA:2853:C:H2' | 25:RA:2854:G:C8 | 2.53 | 0.42 |
| 25:RA:436:C:H2' | 25:RA:438:G:H8 | 1.84 | 0.42 |
| 25:RA:817:C:H2' | 25:RA:818:G:O4' | 2.19 | 0.42 |
| 27:RD:77:ALA:O | 27:RD:116:GLN:HA | 2.20 | 0.42 |
| 28:RE:101:ARG:HD2 | 28:RE:169:ASN:OD1 | 2.19 | 0.42 |
| 28:RE:36:ARG:NH2 | 28:RE:88:GLY:HA2 | 2.34 | 0.42 |
| 32:RI:49:ALA:HA | 32:RI:52:ARG:HG2 | 2.01 | 0.42 |
| 25:RA:2392:A:C8 | 35:RP:60:MET:HG2 | 2.55 | 0.42 |
| 34:RO:122:LEU:HD13 | 39:RT:72:VAL:HG11 | 2.01 | 0.42 |
| 40:RU:94:ASN:C | 40:RU:96:ALA:H | 2.23 | 0.42 |
| 1:XA:1053:G:N7 | 1:XA:1199:U:H2' | 2.35 | 0.42 |
| 1:XA:1150:U:O4 | 1:XA:1151:A:N6 | 2.52 | 0.42 |
| 1:XA:828:A:H2' | 1:XA:829:G:O4' | 2.20 | 0.42 |
| 2:XB:84:GLU:HG3 | 2:XB:215:LEU:HB3 | 2.01 | 0.42 |
| 2:XB:7:VAL:HG11 | 2:XB:217:ARG:CZ | 2.48 | 0.42 |
| 4:XD:121:VAL:O | 4:XD:134:ASP:HA | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:XJ:7:LYS:HB2 | 10:XJ:97:GLU:HB2 | 2.00 | 0.42 |
| 16:XP:19:ILE:HD11 | 16:XP:73:LEU:HD22 | 2.01 | 0.42 |
| 55:Y9:1:MET:HG3 | 55:Y9:33:LYS:CB | 2.45 | 0.42 |
| 25:YA:1441:G:H2' | 25:YA:1442:G:H8 | 1.84 | 0.42 |
| 25:YA:1766:U:H2' | 25:YA:1767:C:C6 | 2.54 | 0.42 |
| 25:YA:2266:A:H4' | 25:YA:2267:A:N3 | 2.34 | 0.42 |
| 25:YA:2305:A:N1 | 30:YG:154:GLY:N | 2.62 | 0.42 |
| 25:YA:2590:A:H2' | 25:YA:2591:C:H6 | 1.84 | 0.42 |
| 25:YA:2745:C:OP2 | 55:Y9:24:TYR:CZ | 2.72 | 0.42 |
| 25:YA:2755:C:N4 | 55:Y9:2:LYS:C | 2.73 | 0.42 |
| 25:YA:479:A:HO2' | 25:YA:481:G:H8 | 1.66 | 0.42 |
| 25:YA:532:A:H4' | 25:YA:533:G:C8 | 2.54 | 0.42 |
| 25:YA:582:G:H2' | 25:YA:583:G:H8 | 1.83 | 0.42 |
| 25:YA:637:A:OP2 | 35:YP:115:LEU:HB2 | 2.19 | 0.42 |
| 26:YB:23:G:H2' | 26:YB:24:G:C8 | 2.54 | 0.42 |
| 30:YG:3:LEU:HD21 | 50:Y4:25:TYR:CD2 | 2.54 | 0.42 |
| 31:YH:149:ARG:HH12 | 55:Y9:18:ARG:NH1 | 2.17 | 0.42 |
| 31:YH:151:ILE:HG22 | 31:YH:153:LYS:HG2 | 2.00 | 0.42 |
| 38:YS:10:ARG:HG2 | 38:YS:13:ARG:NH2 | 2.34 | 0.42 |
| 40:YU:94:ASN:ND2 | 40:YU:94:ASN:O | 2.48 | 0.42 |
| 42:YW:19:LEU:HD23 | 51:Y5:25:LEU:HG | 2.02 | 0.42 |
| 43:YX:27:THR:HA | 43:YX:80:ILE:HA | 2.02 | 0.42 |
| 1:QA:1009:G:O6 | 1:QA:1020:U:O4 | 2.37 | 0.42 |
| 1:QA:1149:C:H2' | 1:QA:1150:U:H6 | 1.85 | 0.42 |
| 1:QA:955:U:H1' | 1:QA:1227:A:N6 | 2.34 | 0.42 |
| 1:QA:947:G:H4' | 1:QA:1332:A:H2 | 1.84 | 0.42 |
| 1:QA:1410:G:H2' | 1:QA:1411:C:H6 | 1.84 | 0.42 |
| 1:QA:21:G:H2' | 1:QA:22:G:H8 | 1.81 | 0.42 |
| 1:QA:738:C:H2' | 1:QA:739:C:C6 | 2.55 | 0.42 |
| 1:QA:751:U:H2' | 1:QA:752:G:O4' | 2.19 | 0.42 |
| 1:QA:966:G:N2 | 22:QV:35:C:H5' | 2.34 | 0.42 |
| 2:QB:93:VAL:HG11 | 2:QB:97:TRP:CD1 | 2.54 | 0.42 |
| 7:QG:94:ARG:NH1 | 7:QG:98:SER:OG | 2.53 | 0.42 |
| 19:QS:19:VAL:HG21 | 19:QS:44:MET:SD | 2.60 | 0.42 |
| 25:RA:2755:C:H42 | 55:R9:1:MET:N | 2.17 | 0.42 |
| 25:RA:1103:A:H5'' | 25:RA:1104:C:C5 | 2.53 | 0.42 |
| 25:RA:131:G:H2' | 25:RA:132:G:C8 | 2.53 | 0.42 |
| 25:RA:1357:U:H2' | 25:RA:1358:G:O4' | 2.20 | 0.42 |
| 25:RA:2291:U:OP1 | 25:RA:2380:C:O2' | 2.38 | 0.42 |
| 25:RA:2481:G:HO2' | 25:RA:2482:G:P | 2.42 | 0.42 |
| 25:RA:2537:U:H2' | 25:RA:2538:C:C6 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:557:U:H2' | 25:RA:558:G:C8 | 2.55 | 0.42 |
| 29:RF:118:ALA:HB2 | 29:RF:123:LEU:HD22 | 2.01 | 0.42 |
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:NH2 | 2.34 | 0.42 |
| 1:XA:1010:G:H2' | 1:XA:1011:G:H8 | 1.84 | 0.42 |
| 1:XA:1321:C:C3' | 1:XA:1322:C:H5'' | 2.50 | 0.42 |
| 1:XA:1374:A:O2' | 7:XG:28:ASN:HB3 | 2.19 | 0.42 |
| 1:XA:149:A:H2' | 1:XA:150:C:C6 | 2.55 | 0.42 |
| 1:XA:624:C:H2' | 1:XA:625:G:H8 | 1.84 | 0.42 |
| 4:XD:57:ARG:HB3 | 4:XD:206:PHE:HB2 | 1.99 | 0.42 |
| 9:XI:65:VAL:CG2 | 9:XI:73:GLN:HG2 | 2.49 | 0.42 |
| 11:XK:82:VAL:HG11 | 11:XK:95:ILE:HD12 | 2.02 | 0.42 |
| 16:XP:57:ARG:NE | 16:XP:79:VAL:O | 2.53 | 0.42 |
| 50:Y4:61:ARG:HG2 | 50:Y4:61:ARG:O | 2.19 | 0.42 |
| 55:Y9:1:MET:HG3 | 55:Y9:33:LYS:CD | 2.45 | 0.42 |
| 25:YA:1257:C:H2' | 25:YA:1258:C:C6 | 2.55 | 0.42 |
| 25:YA:1292:U:H2' | 25:YA:1293:C:C6 | 2.54 | 0.42 |
| 25:YA:1841:U:C2 | 25:YA:1842:G:C8 | 3.07 | 0.42 |
| 25:YA:2278:A:OP2 | 46:Y0:12:ASN:ND2 | 2.52 | 0.42 |
| 25:YA:2744:G:H4' | 55:Y9:19:ARG:O | 2.20 | 0.42 |
| 25:YA:43:G:H2' | 25:YA:44:A:C8 | 2.54 | 0.42 |
| 26:YB:32:C:C4 | 26:YB:51:G:N2 | 2.87 | 0.42 |
| 27:YD:165:ILE:HA | 27:YD:175:LEU:HD23 | 2.02 | 0.42 |
| 1:QA:1107:C:C4 | 1:QA:1108:G:C8 | 3.07 | 0.42 |
| 1:QA:156:G:H2' | 1:QA:157:G:C8 | 2.54 | 0.42 |
| 1:QA:19:C:H5'' | 5:QE:86:ALA:HB3 | 2.00 | 0.42 |
| 1:QA:607:A:H2' | 1:QA:608:A:O4' | 2.20 | 0.42 |
| 6:QF:10:LEU:HD13 | 6:QF:61:LEU:HD13 | 2.02 | 0.42 |
| 9:QI:121:ARG:NH1 | 9:QI:122:ALA:O | 2.53 | 0.42 |
| 10:QJ:13:HIS:HB3 | 10:QJ:68:HIS:NE2 | 2.34 | 0.42 |
| 50:R4:56:VAL:CG2 | 50:R4:58:ARG:HG3 | 2.50 | 0.42 |
| 25:RA:108:U:H2' | 25:RA:109:G:C8 | 2.55 | 0.42 |
| 25:RA:1458:C:H4' | 25:RA:1459:G:O4' | 2.20 | 0.42 |
| 25:RA:1841:U:H2' | 25:RA:1842:G:H8 | 1.84 | 0.42 |
| 25:RA:2406:U:C2 | 35:RP:72:PRO:HB2 | 2.55 | 0.42 |
| 25:RA:51:G:H8 | 25:RA:51:G:OP2 | 2.03 | 0.42 |
| 25:RA:667:U:H2' | 25:RA:668:G:O4' | 2.19 | 0.42 |
| 25:RA:861:A:N3 | 26:RB:79:C:O2' | 2.50 | 0.42 |
| 27:RD:92:ILE:HD12 | 27:RD:104:TYR:CD2 | 2.55 | 0.42 |
| 27:RD:148:GLU:OE1 | 27:RD:151:LYS:NZ | 2.42 | 0.42 |
| 30:RG:11:TYR:CD1 | 30:RG:176:LEU:HD21 | 2.53 | 0.42 |
| 34:RO:77:ILE:HB | 39:RT:74:ARG:HH11 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2377:A:H4' | 38:RS:111:GLU:O | 2.19 | 0.42 |
| 45:RZ:10:ARG:NH2 | 45:RZ:37:VAL:O | 2.53 | 0.42 |
| 1:XA:1126:U:H1' | 1:XA:1280:A:N7 | 2.35 | 0.42 |
| 1:XA:1161:C:H2' | 1:XA:1162:C:C6 | 2.54 | 0.42 |
| 1:XA:1417:G:C6 | 1:XA:1482:G:C6 | 3.08 | 0.42 |
| 1:XA:552:U:H2' | 1:XA:553:A:H8 | 1.82 | 0.42 |
| 1:XA:555:C:H2' | 1:XA:556:C:C6 | 2.55 | 0.42 |
| 3:XC:64:VAL:HG12 | 3:XC:66:VAL:HG23 | 2.02 | 0.42 |
| 13:XM:7:VAL:HG11 | 30:YG:115:ARG:HH12 | 1.85 | 0.42 |
| 22:XV:20:G:H4' | 22:XV:21:U:OP2 | 2.17 | 0.42 |
| 22:XW:28:U:H2' | 22:XW:29:C:C6 | 2.53 | 0.42 |
| 25:YA:1142(A):A:C4 | 25:YA:1144:G:N7 | 2.88 | 0.42 |
| 25:YA:1296:G:OP1 | 25:YA:2709:G:O2' | 2.22 | 0.42 |
| 25:YA:2235:G:H2' | 25:YA:2236:C:C6 | 2.55 | 0.42 |
| 25:YA:2061:G:H5'' | 25:YA:2503:A:C2 | 2.55 | 0.42 |
| 25:YA:269:U:H1' | 25:YA:424:G:N2 | 2.34 | 0.42 |
| 25:YA:270(I):G:H2' | 25:YA:270(J):G:C8 | 2.55 | 0.42 |
| 25:YA:671:C:H2' | 25:YA:672:C:C6 | 2.55 | 0.42 |
| 28:YE:116:VAL:HG23 | 28:YE:157:ALA:HB2 | 2.01 | 0.42 |
| 29:YF:176:LEU:HD21 | 29:YF:181:LEU:HA | 2.02 | 0.42 |
| 32:YI:99:GLU:OE2 | 32:YI:103:ARG:NH2 | 2.52 | 0.42 |
| 32:YI:68:LEU:HA | 32:YI:71:ILE:HG22 | 2.01 | 0.42 |
| 34:YO:103:ALA:HA | 34:YO:122:LEU:O | 2.19 | 0.42 |
| 34:YO:78:ARG:NE | 39:YT:73:GLU:OE1 | 2.52 | 0.42 |
| 35:YP:57:THR:C | 35:YP:59:LEU:N | 2.71 | 0.42 |
| 38:YS:26:LEU:HD22 | 38:YS:87:PHE:HD1 | 1.84 | 0.42 |
| 26:YB:7:G:H4' | 38:YS:29:PHE:CG | 2.54 | 0.42 |
| 38:YS:14:VAL:HG11 | 38:YS:90:GLY:O | 2.19 | 0.42 |
| 39:YT:57:PHE:CG | 39:YT:58:ASN:N | 2.88 | 0.42 |
| 40:YU:92:ARG:NH1 | 40:YU:94:ASN:OD1 | 2.53 | 0.42 |
| 1:QA:1121:U:H2' | 1:QA:1122:U:H6 | 1.85 | 0.42 |
| 1:QA:1347:G:O2' | 1:QA:1348:U:P | 2.78 | 0.42 |
| 1:QA:1352:C:H2' | 1:QA:1353:G:C8 | 2.55 | 0.42 |
| 1:QA:181:G:H4' | 1:QA:182:U:H5' | 2.01 | 0.42 |
| 1:QA:322:C:H2' | 1:QA:323:U:C6 | 2.54 | 0.42 |
| 1:QA:652:U:H1' | 1:QA:653:A:H2 | 1.84 | 0.42 |
| 2:QB:163:PHE:HA | 2:QB:185:ILE:O | 2.19 | 0.42 |
| 2:QB:237:ALA:O | 2:QB:239:VAL:HG23 | 2.19 | 0.42 |
| 4:QD:121:VAL:O | 4:QD:134:ASP:HA | 2.20 | 0.42 |
| 4:QD:63:LYS:HE3 | 4:QD:198:VAL:HG22 | 2.01 | 0.42 |
| 9:QI:96:LEU:HD12 | 9:QI:101:PHE:HB2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1198:U:C2 | 25:RA:1199:U:C5 | 3.08 | 0.42 |
| 25:RA:1588:C:H2' | 25:RA:1589:C:H6 | 1.84 | 0.42 |
| 25:RA:177:G:H5' | 25:RA:178:G:N7 | 2.34 | 0.42 |
| 25:RA:2455:G:C4 | 25:RA:2456:C:C5 | 3.07 | 0.42 |
| 25:RA:2514:U:H2' | 25:RA:2515:C:H6 | 1.85 | 0.42 |
| 25:RA:363(E):U:H3' | 25:RA:363(F):A:C8 | 2.54 | 0.42 |
| 25:RA:740:U:H2' | 25:RA:741:G:C8 | 2.54 | 0.42 |
| 25:RA:746:A:H2' | 25:RA:2612:C:H5'' | 2.01 | 0.42 |
| 25:RA:863:A:H2' | 25:RA:864:G:C8 | 2.55 | 0.42 |
| 27:RD:14:ARG:HG3 | 27:RD:15:PHE:CD1 | 2.55 | 0.42 |
| 27:RD:52:ARG:HE | 27:RD:53:PHE:HE2 | 1.68 | 0.42 |
| 29:RF:155:LEU:HD23 | 29:RF:186:ILE:HD13 | 2.02 | 0.42 |
| 36:RQ:3:MET:HB2 | 36:RQ:93:TYR:CE2 | 2.54 | 0.42 |
| 1:XA:1179:A:H2' | 1:XA:1180:A:O4' | 2.20 | 0.42 |
| 1:XA:1392:G:H2' | 1:XA:1393:U:C6 | 2.54 | 0.42 |
| 1:XA:1496:C:H2' | 1:XA:1497:G:C8 | 2.55 | 0.42 |
| 1:XA:485:G:O2' | 1:XA:486:U:P | 2.78 | 0.42 |
| 1:XA:498:A:O3' | 1:XA:500:G:H8 | 2.02 | 0.42 |
| 1:XA:62:U:OP1 | 1:XA:385:C:O2' | 2.37 | 0.42 |
| 1:XA:864:A:H2' | 1:XA:865:A:C8 | 2.54 | 0.42 |
| 1:XA:950:U:H2' | 1:XA:951:G:H8 | 1.84 | 0.42 |
| 2:XB:164:VAL:HG12 | 2:XB:166:ASP:H | 1.84 | 0.42 |
| 3:XC:129:ALA:HB3 | 3:XC:132:ARG:HB3 | 2.02 | 0.42 |
| 1:XA:932:C:H5' | 7:XG:4:ARG:HG3 | 2.02 | 0.42 |
| 8:XH:104:ARG:HD2 | 8:XH:138:TRP:CE3 | 2.54 | 0.42 |
| 12:XL:39:VAL:HB | 12:XL:57:LYS:HB2 | 2.01 | 0.42 |
| 13:XM:65:LYS:HB3 | 50:Y4:50:VAL:HG21 | 2.02 | 0.42 |
| 19:XS:10:PHE:HE1 | 19:XS:15:LEU:HD21 | 1.84 | 0.42 |
| 1:XA:1319:A:OP1 | 19:XS:3:ARG:HD3 | 2.20 | 0.42 |
| 22:XV:53:G:HO2' | 22:XV:54:G:P | 2.41 | 0.42 |
| 25:YA:1842:G:O2' | 27:YD:253:GLN:NE2 | 2.47 | 0.42 |
| 25:YA:2153:G:H2' | 25:YA:2154:G:H8 | 1.84 | 0.42 |
| 25:YA:270(P):C:H2' | 25:YA:270(Q):C:H6 | 1.85 | 0.42 |
| 25:YA:278:A:O2' | 25:YA:279:C:O4' | 2.34 | 0.42 |
| 25:YA:459:U:H2' | 25:YA:460:A:H8 | 1.84 | 0.42 |
| 26:YB:111:U:H2' | 26:YB:112:G:C8 | 2.55 | 0.42 |
| 29:YF:178:PRO:HB3 | 29:YF:198:ALA:HB2 | 2.00 | 0.42 |
| 30:YG:16:ARG:O | 30:YG:20:ILE:HG12 | 2.19 | 0.42 |
| 41:YV:34:GLU:O | 41:YV:36:PRO:HD3 | 2.20 | 0.42 |
| 1:QA:1211:U:H5' | 1:QA:1212:U:OP1 | 2.20 | 0.42 |
| 1:QA:1419:G:H1 | 1:QA:1481:U:H3 | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:392:G:H2' | 1:QA:393:A:C8 | 2.55 | 0.42 |
| 1:QA:429:U:H3' | 4:QD:9:CYS:SG | 2.60 | 0.42 |
| 1:QA:446:G:H2' | 1:QA:447:G:O4' | 2.20 | 0.42 |
| 1:QA:629:G:H2' | 1:QA:630:G:C8 | 2.55 | 0.42 |
| 1:QA:658:G:H2' | 1:QA:659:U:C6 | 2.55 | 0.42 |
| 1:QA:667:G:H2' | 1:QA:668:G:H8 | 1.84 | 0.42 |
| 2:QB:48:MET:HA | 2:QB:51:LEU:HD12 | 2.02 | 0.42 |
| 12:QL:104:VAL:HG12 | 12:QL:105:TYR:CD2 | 2.54 | 0.42 |
| 13:QM:13:LYS:HA | 13:QM:44:ARG:HD2 | 2.02 | 0.42 |
| 54:R8:34:TRP:CE3 | 54:R8:35:GLN:HB2 | 2.55 | 0.42 |
| 55:R9:25:VAL:O | 55:R9:33:LYS:HA | 2.19 | 0.42 |
| 25:RA:1475:G:H2' | 25:RA:1476:C:C6 | 2.54 | 0.42 |
| 25:RA:150:C:H2' | 25:RA:151:C:H6 | 1.84 | 0.42 |
| 25:RA:1680:U:H2' | 25:RA:1681:G:O4' | 2.20 | 0.42 |
| 25:RA:17:G:HO2' | 40:RU:25:TRP:HD1 | 1.68 | 0.42 |
| 25:RA:2285:C:N4 | 52:R6:24:GLU:OE2 | 2.52 | 0.42 |
| 25:RA:2379:G:H2' | 25:RA:2380:C:H6 | 1.85 | 0.42 |
| 25:RA:2532:G:N2 | 25:RA:2663:G:O2' | 2.53 | 0.42 |
| 25:RA:2758:A:C4 | 31:RH:67:LEU:HD21 | 2.54 | 0.42 |
| 25:RA:621:A:OP2 | 35:RP:108:LYS:NZ | 2.52 | 0.42 |
| 25:RA:783:A:H2' | 25:RA:784:A:H4' | 2.00 | 0.42 |
| 26:RB:16:G:N2 | 26:RB:69:G:H1' | 2.35 | 0.42 |
| 27:RD:4:LYS:NZ | 27:RD:20:ASP:HA | 2.35 | 0.42 |
| 31:RH:14:GLY:O | 31:RH:29:PRO:HD3 | 2.20 | 0.42 |
| 34:RO:2:ILE:HG21 | 34:RO:8:LEU:HD21 | 2.02 | 0.42 |
| 36:RQ:62:GLY:HA3 | 36:RQ:107:ALA:O | 2.20 | 0.42 |
| 1:XA:1129:C:H4' | 1:XA:1130:A:H5' | 2.01 | 0.42 |
| 1:XA:1264:C:H2' | 1:XA:1265:G:H8 | 1.83 | 0.42 |
| 1:XA:1369:C:H2' | 1:XA:1370:G:C8 | 2.55 | 0.42 |
| 1:XA:1414:U:H2' | 1:XA:1415:G:C8 | 2.54 | 0.42 |
| 1:XA:164:U:H2' | 1:XA:165:C:C6 | 2.54 | 0.42 |
| 1:XA:295:C:H2' | 1:XA:296:U:O4' | 2.20 | 0.42 |
| 1:XA:560:U:H4' | 1:XA:561:U:C5' | 2.50 | 0.42 |
| 1:XA:812:C:H4' | 1:XA:813:U:H5' | 2.02 | 0.42 |
| 1:XA:745:C:OP1 | 1:XA:851:G:O2' | 2.37 | 0.42 |
| 1:XA:902:G:H2' | 1:XA:903:G:H8 | 1.84 | 0.42 |
| 1:XA:412:A:H61 | 4:XD:35:ARG:HA | 1.84 | 0.42 |
| 22:XV:20:G:H5' | 22:XV:21:U:C5 | 2.54 | 0.42 |
| 50:Y4:55:ARG:HD3 | 50:Y4:58:ARG:NH2 | 2.35 | 0.42 |
| 55:Y9:32:HIS:C | 55:Y9:34:GLN:H | 2.23 | 0.42 |
| 25:YA:1026:U:H4' | 25:YA:1027:A:OP1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:137(A):G:H2' | 25:YA:139:G:N7 | 2.34 | 0.42 |
| 25:YA:817:C:O2' | 25:YA:839:U:OP1 | 2.25 | 0.42 |
| 45:YZ:151:HIS:CB | 45:YZ:170:THR:HA | 2.50 | 0.42 |
| 1:QA:113:G:H1' | 1:QA:354:G:H5' | 2.01 | 0.42 |
| 1:QA:1298:C:H4' | 1:QA:1299:A:C5 | 2.55 | 0.42 |
| 1:QA:1343:G:H4' | 9:QL:122:ALA:HB3 | 2.00 | 0.42 |
| 1:QA:513:C:H2' | 1:QA:514:C:H6 | 1.85 | 0.42 |
| 1:QA:677:U:O2 | 1:QA:777:A:O2' | 2.36 | 0.42 |
| 1:QA:763:G:H2' | 1:QA:764:C:H6 | 1.85 | 0.42 |
| 2:QB:12:GLU:HA | 2:QB:16:HIS:CD2 | 2.55 | 0.42 |
| 1:QA:1160:G:H4' | 2:QB:132:LYS:NZ | 2.34 | 0.42 |
| 18:QR:47:THR:O | 18:QR:83:GLU:N | 2.52 | 0.42 |
| 25:RA:1032:A:O2' | 25:RA:1033:U:P | 2.78 | 0.42 |
| 25:RA:1094:U:O2' | 25:RA:1096:A:OP1 | 2.29 | 0.42 |
| 25:RA:1116:C:H2' | 25:RA:1117:G:C8 | 2.55 | 0.42 |
| 25:RA:693:C:O2' | 25:RA:1353:A:N3 | 2.48 | 0.42 |
| 25:RA:1540:G:H2' | 25:RA:1541:U:C6 | 2.55 | 0.42 |
| 25:RA:1530:G:H1 | 25:RA:1541:U:H3 | 1.67 | 0.42 |
| 25:RA:220:G:H21 | 25:RA:429:A:N6 | 2.17 | 0.42 |
| 25:RA:2368:C:H2' | 25:RA:2369:A:C8 | 2.53 | 0.42 |
| 25:RA:2475:C:H42 | 25:RA:2529:G:H22 | 1.67 | 0.42 |
| 25:RA:2543:G:H2' | 25:RA:2544:G:C8 | 2.55 | 0.42 |
| 25:RA:2838:G:C4 | 25:RA:2839:G:C8 | 3.07 | 0.42 |
| 25:RA:81:G:C6 | 25:RA:82:G:N2 | 2.87 | 0.42 |
| 27:RD:27:THR:HG21 | 27:RD:81:ALA:HB1 | 2.01 | 0.42 |
| 28:RE:74:PRO:HG2 | 28:RE:77:ILE:HG22 | 2.02 | 0.42 |
| 34:RO:64:ARG:HB2 | 34:RO:83:ALA:HB3 | 2.01 | 0.42 |
| 25:RA:661:C:H5'' | 35:RP:15:ARG:NH2 | 2.35 | 0.42 |
| 35:RP:61:ARG:HG3 | 54:R8:13:ARG:CD | 2.49 | 0.42 |
| 25:RA:2020:A:H4' | 40:RU:25:TRP:HZ3 | 1.85 | 0.42 |
| 45:RZ:103:ARG:HD3 | 45:RZ:136:PHE:CD2 | 2.55 | 0.42 |
| 1:XA:1016:A:H2' | 1:XA:1017:G:O4' | 2.20 | 0.42 |
| 1:XA:1038:C:H2' | 1:XA:1039:C:C6 | 2.55 | 0.42 |
| 1:XA:109:A:C6 | 1:XA:326:G:C6 | 3.08 | 0.42 |
| 1:XA:358:U:H2' | 1:XA:359:U:C6 | 2.55 | 0.42 |
| 1:XA:807:A:H2' | 1:XA:808:C:H6 | 1.83 | 0.42 |
| 3:XC:20:SER:OG | 3:XC:22:TRP:NE1 | 2.53 | 0.42 |
| 4:XD:105:VAL:HG13 | 4:XD:110:PHE:HB2 | 2.02 | 0.42 |
| 13:XM:83:ASP:H | 13:XM:93:ARG:NH2 | 2.17 | 0.42 |
| 14:YN:23:ARG:NH1 | 14:YN:30:ALA:HB2 | 2.34 | 0.42 |
| 25:YA:2527:C:H5' | 55:Y9:14:CYS:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:2660:A:H2' | 25:YA:2661:G:O4' | 2.20 | 0.42 |
| 25:YA:2742:C:O2' | 55:Y9:25:VAL:C | 2.57 | 0.42 |
| 25:YA:65:C:H2' | 25:YA:66:C:H6 | 1.85 | 0.42 |
| 25:YA:689:A:H2' | 25:YA:690:G:H8 | 1.85 | 0.42 |
| 26:YB:3:C:H2' | 26:YB:4:C:C6 | 2.54 | 0.42 |
| 27:YD:10:THR:OG1 | 27:YD:13:ARG:HG3 | 2.19 | 0.42 |
| 31:YH:148:ILE:HG23 | 55:Y9:20:HIS:NE2 | 2.35 | 0.42 |
| 35:YP:82:GLY:HA2 | 35:YP:113:LYS:O | 2.20 | 0.42 |
| 1:QA:1031:G:H8 | 1:QA:1031:G:OP2 | 2.03 | 0.42 |
| 1:QA:1060:C:H2' | 1:QA:1061:G:H8 | 1.85 | 0.42 |
| 1:QA:864:A:O2' | 1:QA:1078:U:O4 | 2.20 | 0.42 |
| 1:QA:1435:G:H2' | 1:QA:1436:U:C6 | 2.55 | 0.42 |
| 1:QA:148:G:H2' | 1:QA:149:A:C8 | 2.54 | 0.42 |
| 1:QA:672:U:H3 | 1:QA:734:G:H1 | 1.68 | 0.42 |
| 1:QA:757:U:H2' | 1:QA:758:G:O4' | 2.19 | 0.42 |
| 3:QC:186:PHE:HA | 3:QC:198:VAL:O | 2.20 | 0.42 |
| 3:QC:52:LEU:H | 3:QC:52:LEU:HD23 | 1.85 | 0.42 |
| 3:QC:5:ILE:HD11 | 14:QN:49:HIS:HE1 | 1.84 | 0.42 |
| 4:QD:127:THR:HA | 4:QD:132:ARG:HA | 2.02 | 0.42 |
| 6:QF:7:ASN:HB2 | 6:QF:89:MET:HB3 | 2.02 | 0.42 |
| 7:QG:15:ASP:H | 7:QG:20:ASP:H | 1.68 | 0.42 |
| 25:RA:1790:C:H2' | 25:RA:1791:A:C8 | 2.55 | 0.42 |
| 25:RA:2372:G:H2' | 25:RA:2373:G:H8 | 1.84 | 0.42 |
| 25:RA:2747:G:O6 | 25:RA:2754:U:H3' | 2.20 | 0.42 |
| 25:RA:2869:G:H2' | 25:RA:2870:C:C6 | 2.55 | 0.42 |
| 25:RA:823:G:H2' | 25:RA:824:A:C8 | 2.54 | 0.42 |
| 40:RU:90:VAL:HG11 | 41:RV:40:LEU:HG | 2.02 | 0.42 |
| 43:RX:70:LEU:H | 43:RX:70:LEU:HD23 | 1.84 | 0.42 |
| 1:XA:1171:G:H2' | 1:XA:1172:C:C6 | 2.54 | 0.42 |
| 1:XA:1262:C:H2' | 1:XA:1263:C:C6 | 2.55 | 0.42 |
| 1:XA:1323:G:H2' | 1:XA:1324:A:C8 | 2.54 | 0.42 |
| 1:XA:582:U:H2' | 1:XA:583:A:H8 | 1.85 | 0.42 |
| 1:XA:584:G:H2' | 1:XA:585:G:H8 | 1.84 | 0.42 |
| 2:XB:167:PRO:HG2 | 2:XB:192:SER:CB | 2.49 | 0.42 |
| 4:XD:173:TRP:CZ3 | 4:XD:193:ASP:HB3 | 2.55 | 0.42 |
| 5:XE:51:VAL:HB | 5:XE:52:PRO:HD3 | 2.02 | 0.42 |
| 9:XI:7:THR:O | 9:XI:83:ARG:HD2 | 2.20 | 0.42 |
| 25:YA:1246:A:OP1 | 35:YP:15:ARG:NH2 | 2.45 | 0.42 |
| 25:YA:1424:G:H2' | 25:YA:1425:G:O4' | 2.20 | 0.42 |
| 25:YA:1470:G:O2' | 25:YA:1522:G:O6 | 2.22 | 0.42 |
| 25:YA:1550:C:OP1 | 25:YA:1727:U:O2' | 2.24 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:185:U:H2' | 25:YA:186:G:C8 | 2.55 | 0.42 |
| 25:YA:217:G:C4 | 25:YA:218:A:C8 | 3.08 | 0.42 |
| 25:YA:1669:A:O3' | 25:YA:2549:G:H5' | 2.20 | 0.42 |
| 25:YA:376:C:H2' | 25:YA:377:C:H6 | 1.85 | 0.42 |
| 25:YA:881:G:O6 | 25:YA:895:U:O2 | 2.38 | 0.42 |
| 27:YD:71:ASP:HB2 | 27:YD:103:ARG:HH12 | 1.85 | 0.42 |
| 27:YD:122:ASP:CG | 27:YD:123:ALA:H | 2.21 | 0.42 |
| 33:YN:13:TRP:HB2 | 33:YN:133:GLN:HB3 | 2.01 | 0.42 |
| 33:YN:18:ALA:HB2 | 33:YN:54:VAL:HG13 | 2.01 | 0.42 |
| 36:YQ:74:TYR:HD2 | 36:YQ:91:GLU:HB3 | 1.85 | 0.42 |
| 1:QA:1167:A:H2' | 1:QA:1169:A:C8 | 2.55 | 0.41 |
| 1:QA:1443:G:H5' | 1:QA:1446:A:OP2 | 2.20 | 0.41 |
| 1:QA:267:C:P | 17:QQ:67:LYS:HD2 | 2.59 | 0.41 |
| 9:QI:83:ARG:O | 9:QI:86:VAL:HG12 | 2.20 | 0.41 |
| 15:QO:36:ILE:HG23 | 15:QO:56:LEU:HD11 | 2.02 | 0.41 |
| 16:QP:19:ILE:HD11 | 16:QP:73:LEU:HD22 | 2.02 | 0.41 |
| 24:QY:40:C:H2' | 24:QY:41:C:C6 | 2.55 | 0.41 |
| 25:RA:30:G:O2' | 25:RA:1214:A:N3 | 2.36 | 0.41 |
| 25:RA:1259:G:H2' | 25:RA:1260:G:C8 | 2.55 | 0.41 |
| 25:RA:2011:U:H2' | 25:RA:2012:G:O4' | 2.19 | 0.41 |
| 25:RA:2472:G:N1 | 25:RA:2477:C:OP1 | 2.38 | 0.41 |
| 25:RA:270(G):C:H2' | 25:RA:270(H):C:C6 | 2.55 | 0.41 |
| 25:RA:784:A:O2' | 25:RA:785:G:H5'' | 2.20 | 0.41 |
| 27:RD:24:ILE:HD13 | 27:RD:82:ILE:HG22 | 2.01 | 0.41 |
| 27:RD:30:GLU:CD | 27:RD:63:ARG:HE | 2.23 | 0.41 |
| 29:RF:32:LEU:HA | 29:RF:32:LEU:HD12 | 1.87 | 0.41 |
| 31:RH:86:GLU:HG3 | 31:RH:164:TYR:HD1 | 1.84 | 0.41 |
| 35:RP:144:GLU:HA | 35:RP:145:PRO:HD3 | 1.87 | 0.41 |
| 36:RQ:55:VAL:HG13 | 45:RZ:178:GLU:HB3 | 2.02 | 0.41 |
| 38:RS:110:LEU:HB3 | 38:RS:112:PHE:CE1 | 2.55 | 0.41 |
| 40:RU:59:ARG:O | 40:RU:63:VAL:HG23 | 2.20 | 0.41 |
| 1:XA:1291:G:H2' | 1:XA:1292:U:C6 | 2.55 | 0.41 |
| 8:XH:12:ARG:HH12 | 8:XH:27:PRO:HD3 | 1.85 | 0.41 |
| 10:XJ:38:ILE:O | 10:XJ:38:ILE:HG13 | 2.20 | 0.41 |
| 19:XS:26:GLY:O | 19:XS:27:GLU:HG2 | 2.20 | 0.41 |
| 20:XT:30:LYS:HZ2 | 20:XT:80:ARG:NH1 | 2.18 | 0.41 |
| 22:XW:25:U:H2' | 22:XW:26:C:C6 | 2.55 | 0.41 |
| 47:Y1:3:LYS:O | 47:Y1:12:PRO:HD3 | 2.20 | 0.41 |
| 25:YA:84:A:H2 | 25:YA:103:A:C5 | 2.37 | 0.41 |
| 25:YA:1844:C:H2' | 25:YA:1845:G:C8 | 2.53 | 0.41 |
| 25:YA:2746:U:H2' | 25:YA:2747:G:C8 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:2757:A:N3 | 25:YA:2757:A:H2' | 2.35 | 0.41 |
| 25:YA:2809:A:H2' | 25:YA:2810:A:H8 | 1.85 | 0.41 |
| 26:YB:17:C:H2' | 26:YB:18:G:O4' | 2.20 | 0.41 |
| 35:YP:97:PRO:C | 35:YP:99:LEU:H | 2.22 | 0.41 |
| 38:YS:14:VAL:O | 38:YS:18:ILE:HG12 | 2.20 | 0.41 |
| 38:YS:20:ARG:HH22 | 46:Y0:47:PRO:HB2 | 1.84 | 0.41 |
| 43:YX:31:HIS:CE1 | 43:YX:33:LYS:HB2 | 2.55 | 0.41 |
| 44:YY:15:VAL:HG21 | 44:YY:42:VAL:HG11 | 2.01 | 0.41 |
| 1:QA:1226:C:H42 | 13:QM:104:ARG:NH1 | 2.18 | 0.41 |
| 1:QA:1513:A:H2' | 1:QA:1514:C:H6 | 1.86 | 0.41 |
| 1:QA:464:G:N1 | 1:QA:467:G:OP2 | 2.54 | 0.41 |
| 1:QA:962:C:H1' | 1:QA:1201:A:N6 | 2.34 | 0.41 |
| 1:QA:363:A:N1 | 12:QL:31:PRO:HD2 | 2.35 | 0.41 |
| 9:QI:111:ARG:HG3 | 14:QN:61:TRP:CD1 | 2.55 | 0.41 |
| 22:QV:28:U:H2' | 22:QV:29:C:H6 | 1.84 | 0.41 |
| 22:QV:37:U:H2' | 22:QV:38:A:H8 | 1.85 | 0.41 |
| 46:R0:15:ASP:OD1 | 46:R0:16:SER:N | 2.53 | 0.41 |
| 25:RA:1201:C:C2 | 25:RA:1202:C:C5 | 3.08 | 0.41 |
| 25:RA:1351:C:H2' | 25:RA:1352:U:C6 | 2.55 | 0.41 |
| 25:RA:1569:A:H2' | 25:RA:1570:A:C8 | 2.54 | 0.41 |
| 25:RA:2078:C:H2' | 25:RA:2079:U:C6 | 2.55 | 0.41 |
| 25:RA:2868:A:H2' | 25:RA:2869:G:C8 | 2.55 | 0.41 |
| 28:RE:6:GLY:HA2 | 28:RE:51:PHE:CE1 | 2.55 | 0.41 |
| 30:RG:16:ARG:O | 30:RG:20:ILE:HG12 | 2.20 | 0.41 |
| 31:RH:154:PRO:HB3 | 31:RH:162:ILE:O | 2.20 | 0.41 |
| 33:RN:73:THR:HB | 33:RN:82:LEU:HD11 | 2.02 | 0.41 |
| 37:RR:86:ARG:NH2 | 37:RR:118:GLU:OXT | 2.52 | 0.41 |
| 40:RU:44:ASN:ND2 | 41:RV:75:PHE:HB3 | 2.35 | 0.41 |
| 43:RX:31:HIS:HB3 | 43:RX:34:ALA:HB2 | 2.02 | 0.41 |
| 1:XA:1254:C:H2' | 1:XA:1255:G:C8 | 2.54 | 0.41 |
| 1:XA:235:C:H2' | 1:XA:236:G:H8 | 1.84 | 0.41 |
| 1:XA:314:C:H2' | 1:XA:315:A:C8 | 2.55 | 0.41 |
| 1:XA:41:G:C6 | 1:XA:402:G:C6 | 3.09 | 0.41 |
| 1:XA:784:C:H2' | 1:XA:785:G:C8 | 2.55 | 0.41 |
| 5:XE:15:ARG:HG3 | 5:XE:28:PHE:CE1 | 2.54 | 0.41 |
| 7:XG:45:ASP:O | 7:XG:49:ILE:HG12 | 2.20 | 0.41 |
| 1:XA:377:G:OP1 | 16:XP:3:LYS:HD2 | 2.19 | 0.41 |
| 18:XR:44:LEU:HD21 | 18:XR:74:ARG:HH21 | 1.85 | 0.41 |
| 22:XW:19:G:H1' | 22:XW:59:A:C2 | 2.56 | 0.41 |
| 47:Y1:76:ARG:HD2 | 47:Y1:76:ARG:N | 2.35 | 0.41 |
| 25:YA:1354:A:H5' | 27:YD:38:LYS:NZ | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1479:G:N7 | 25:YA:1510:A:N6 | 2.68 | 0.41 |
| 25:YA:1550:C:H2' | 25:YA:1551:C:H6 | 1.84 | 0.41 |
| 25:YA:1812:A:H4' | 27:YD:46:GLN:HE22 | 1.85 | 0.41 |
| 25:YA:1835:G:N3 | 25:YA:1835:G:H2' | 2.35 | 0.41 |
| 25:YA:2774:C:H2' | 25:YA:2775:A:O4' | 2.19 | 0.41 |
| 25:YA:27:G:N2 | 25:YA:513:A:OP2 | 2.52 | 0.41 |
| 25:YA:689:A:H2' | 25:YA:690:G:C8 | 2.55 | 0.41 |
| 25:YA:710:G:H2' | 25:YA:711:G:H8 | 1.85 | 0.41 |
| 25:YA:922:U:H2' | 25:YA:923:C:C6 | 2.55 | 0.41 |
| 26:YB:28:C:OP2 | 38:YS:33:LYS:HE3 | 2.21 | 0.41 |
| 30:YG:72:ARG:HD3 | 30:YG:87:PRO:HB3 | 2.02 | 0.41 |
| 33:YN:30:ILE:HD13 | 33:YN:99:LEU:HD11 | 2.01 | 0.41 |
| 35:YP:107:LYS:O | 35:YP:109:GLY:N | 2.54 | 0.41 |
| 36:YQ:34:LEU:HB2 | 36:YQ:118:LEU:HD22 | 2.01 | 0.41 |
| 45:YZ:99:TYR:CE1 | 45:YZ:125:LEU:HB2 | 2.54 | 0.41 |
| 1:QA:1151:A:H2' | 1:QA:1152:A:H8 | 1.85 | 0.41 |
| 1:QA:161:A:H2' | 1:QA:162:A:C8 | 2.56 | 0.41 |
| 1:QA:1103:C:O2 | 2:QB:107:THR:HG21 | 2.21 | 0.41 |
| 3:QC:81:GLY:HA2 | 3:QC:84:ILE:HG22 | 2.03 | 0.41 |
| 11:QK:124:LYS:HE3 | 11:QK:125:PHE:CE1 | 2.56 | 0.41 |
| 25:RA:1664:A:H61 | 25:RA:1996:C:N4 | 2.17 | 0.41 |
| 25:RA:1829:A:H3' | 25:RA:1830:C:H6 | 1.85 | 0.41 |
| 25:RA:2291:U:O2' | 25:RA:2374:C:O2 | 2.35 | 0.41 |
| 25:RA:300:A:H2' | 25:RA:334:C:H1' | 2.02 | 0.41 |
| 25:RA:399:G:H2' | 25:RA:400:G:O4' | 2.21 | 0.41 |
| 25:RA:523:C:O2 | 25:RA:553:U:O2' | 2.34 | 0.41 |
| 25:RA:639:U:C2 | 25:RA:640:C:C5 | 3.08 | 0.41 |
| 25:RA:669:G:H5'' | 25:RA:670:A:OP2 | 2.20 | 0.41 |
| 25:RA:752:A:H4' | 25:RA:753:C:H5' | 2.02 | 0.41 |
| 27:RD:260:ARG:NH2 | 27:RD:264:LYS:HD3 | 2.36 | 0.41 |
| 36:RQ:66:ILE:HG13 | 36:RQ:67:ARG:N | 2.35 | 0.41 |
| 38:RS:27:SER:HA | 38:RS:88:ASP:HB3 | 2.02 | 0.41 |
| 1:XA:1347:G:O2' | 1:XA:1348:U:H5 | 2.03 | 0.41 |
| 1:XA:272:C:C2 | 1:XA:273:A:C8 | 3.08 | 0.41 |
| 1:XA:452:A:O2' | 16:XP:72:ARG:HD2 | 2.21 | 0.41 |
| 1:XA:770:C:H2' | 1:XA:771:G:H8 | 1.85 | 0.41 |
| 2:XB:93:VAL:HG11 | 2:XB:97:TRP:CD1 | 2.55 | 0.41 |
| 1:XA:737:A:H5' | 6:XF:90:VAL:O | 2.21 | 0.41 |
| 55:Y9:13:LYS:HA | 55:Y9:13:LYS:HD3 | 1.79 | 0.41 |
| 25:YA:1291:C:H2' | 25:YA:1292:U:H6 | 1.85 | 0.41 |
| 25:YA:2011:U:H2' | 25:YA:2012:G:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 25:YA:2030:A:H4' | 25:YA:2031:A:C8 | 2.54 | 0.41 |
| 25:YA:463:G:N2 | 25:YA:466:A:OP2 | 2.30 | 0.41 |
| 25:YA:816:C:H2' | 25:YA:817:C:H6 | 1.85 | 0.41 |
| 25:YA:995:C:O2 | 33:YN:3:THR:OG1 | 2.30 | 0.41 |
| 26:YB:48:A:H2' | 26:YB:49:C:C6 | 2.55 | 0.41 |
| 31:YH:149:ARG:HD3 | 31:YH:162:ILE:HD12 | 2.02 | 0.41 |
| 1:QA:1152:A:H2' | 1:QA:1153:C:C6 | 2.55 | 0.41 |
| 1:QA:1242:C:H2' | 1:QA:1243:C:C6 | 2.55 | 0.41 |
| 1:QA:1289:A:H2' | 1:QA:1290:G:H5' | 2.03 | 0.41 |
| 1:QA:1349:A:H62 | 1:QA:1373:G:H21 | 1.66 | 0.41 |
| 1:QA:287:U:H2' | 1:QA:288:A:C8 | 2.55 | 0.41 |
| 1:QA:642:A:N7 | 8:QH:115:SER:HA | 2.35 | 0.41 |
| 1:QA:784:C:H2' | 1:QA:785:G:H8 | 1.85 | 0.41 |
| 1:QA:792:A:H2' | 1:QA:792:A:N3 | 2.35 | 0.41 |
| 1:QA:812:C:H1' | 1:QA:813:U:OP2 | 2.21 | 0.41 |
| 1:QA:913:A:H4' | 1:QA:914:A:O5' | 2.21 | 0.41 |
| 2:QB:97:TRP:NE1 | 2:QB:101:MET:HG3 | 2.36 | 0.41 |
| 11:QK:29:ILE:HG13 | 11:QK:44:SER:HB3 | 2.01 | 0.41 |
| 20:QT:43:LEU:HD13 | 20:QT:51:GLU:HG3 | 2.03 | 0.41 |
| 49:R3:3:ARG:NH2 | 49:R3:60:GLU:OXT | 2.53 | 0.41 |
| 25:RA:1676:A:H2' | 25:RA:1677:A:O4' | 2.20 | 0.41 |
| 25:RA:1819:A:H4' | 25:RA:1820:U:O5' | 2.19 | 0.41 |
| 25:RA:2108:C:H2' | 25:RA:2109:U:H6 | 1.85 | 0.41 |
| 25:RA:2359:C:H2' | 25:RA:2360:A:O4' | 2.19 | 0.41 |
| 25:RA:2454:G:C2 | 25:RA:2499:C:N4 | 2.88 | 0.41 |
| 25:RA:2061:G:H2' | 25:RA:2501:C:O2' | 2.21 | 0.41 |
| 25:RA:242:G:N2 | 25:RA:254:G:H2' | 2.35 | 0.41 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:C8 | 2.73 | 0.41 |
| 25:RA:2712:U:O2' | 25:RA:2712(A):A:OP1 | 2.33 | 0.41 |
| 25:RA:2754:U:H4' | 55:R9:30:PRO:HD2 | 2.02 | 0.41 |
| 25:RA:809:G:H2' | 25:RA:810:U:C6 | 2.56 | 0.41 |
| 31:RH:28:GLY:HA3 | 31:RH:79:VAL:HB | 2.02 | 0.41 |
| 33:RN:123:TYR:HE2 | 33:RN:129:PRO:HD2 | 1.86 | 0.41 |
| 40:RU:21:ALA:HA | 40:RU:24:TYR:CE2 | 2.56 | 0.41 |
| 41:RV:35:LEU:HD13 | 41:RV:37:VAL:HG23 | 2.02 | 0.41 |
| 1:XA:1015:A:H2' | 1:XA:1016:A:C8 | 2.56 | 0.41 |
| 1:XA:489:C:H2' | 1:XA:490:G:C8 | 2.55 | 0.41 |
| 1:XA:512:U:H2' | 1:XA:513:C:C6 | 2.55 | 0.41 |
| 1:XA:784:C:H2' | 1:XA:785:G:H8 | 1.85 | 0.41 |
| 1:XA:865:A:H2' | 1:XA:866:C:C6 | 2.56 | 0.41 |
| 12:XL:27:LEU:HD13 | 12:XL:62:SER:CB | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:XW:9:G:H4' | 22:XW:47:G:H4' | 2.02 | 0.41 |
| 54:Y8:34:TRP:CE3 | 54:Y8:35:GLN:HB2 | 2.55 | 0.41 |
| 25:YA:1379:A:H4' | 25:YA:1380:G:OP2 | 2.19 | 0.41 |
| 25:YA:141:A:H8 | 25:YA:1408:C:H1' | 1.85 | 0.41 |
| 25:YA:1706:U:O2' | 25:YA:1757:U:H5' | 2.20 | 0.41 |
| 25:YA:1939:U:O2 | 25:YA:1967:C:H4' | 2.20 | 0.41 |
| 25:YA:210:C:H2' | 25:YA:211:A:C8 | 2.55 | 0.41 |
| 25:YA:2526:G:N2 | 25:YA:2537:U:O2 | 2.44 | 0.41 |
| 25:YA:848:G:O6 | 25:YA:929:G:H2' | 2.20 | 0.41 |
| 42:YW:88:ARG:HB2 | 42:YW:92:ARG:HB2 | 2.01 | 0.41 |
| 44:YY:99:CYS:SG | 44:YY:100:ALA:N | 2.94 | 0.41 |
| 45:YZ:145:GLU:HG3 | 45:YZ:146:ILE:N | 2.34 | 0.41 |
| 1:QA:1096:C:H2' | 1:QA:1097:C:C6 | 2.55 | 0.41 |
| 1:QA:174:C:H2' | 1:QA:175:C:C6 | 2.56 | 0.41 |
| 1:QA:551:U:H2' | 1:QA:552:U:C6 | 2.56 | 0.41 |
| 1:QA:639:G:H2' | 1:QA:640:A:C8 | 2.54 | 0.41 |
| 1:QA:726:C:H2' | 1:QA:727:G:C8 | 2.54 | 0.41 |
| 1:QA:97:U:H2' | 1:QA:99:C:C6 | 2.55 | 0.41 |
| 1:QA:1376:U:P | 7:QG:94:ARG:HH22 | 2.43 | 0.41 |
| 16:QP:53:VAL:O | 16:QP:57:ARG:HG2 | 2.20 | 0.41 |
| 22:QW:10:G:C6 | 22:QW:27:G:C5 | 3.09 | 0.41 |
| 22:QW:41:C:H2' | 22:QW:42:C:C6 | 2.55 | 0.41 |
| 52:R6:16:CYS:HB2 | 52:R6:18:ARG:NH1 | 2.36 | 0.41 |
| 25:RA:1405:U:H2' | 25:RA:1406:U:C6 | 2.48 | 0.41 |
| 25:RA:1528:A:C8 | 25:RA:1529:A:C8 | 3.09 | 0.41 |
| 25:RA:1556:C:H2' | 25:RA:1557:C:C6 | 2.56 | 0.41 |
| 25:RA:2506:U:O2 | 25:RA:2506:U:H2' | 2.20 | 0.41 |
| 25:RA:324:A:N6 | 25:RA:339:U:O4' | 2.54 | 0.41 |
| 29:RF:32:LEU:HD23 | 29:RF:112:MET:HE1 | 2.02 | 0.41 |
| 37:RR:96:ARG:NH2 | 37:RR:117:VAL:HG23 | 2.35 | 0.41 |
| 41:RV:52:VAL:HG21 | 41:RV:55:ALA:HB3 | 2.02 | 0.41 |
| 1:XA:1112:C:H1' | 3:XC:179:ARG:NH1 | 2.36 | 0.41 |
| 1:XA:360:A:C6 | 1:XA:361:G:C6 | 3.09 | 0.41 |
| 1:XA:701:C:OP1 | 1:XA:702:A:O2' | 2.22 | 0.41 |
| 1:XA:773:G:O6 | 1:XA:807:A:N6 | 2.53 | 0.41 |
| 2:XB:54:THR:O | 2:XB:58:ILE:HG12 | 2.20 | 0.41 |
| 49:Y3:31:LEU:HA | 49:Y3:31:LEU:HD23 | 1.91 | 0.41 |
| 25:YA:1141:U:H1' | 25:YA:1142(A):A:C5 | 2.56 | 0.41 |
| 25:YA:1344:G:H4' | 25:YA:1384:A:C5 | 2.56 | 0.41 |
| 25:YA:1538:G:H2' | 25:YA:1539:G:H8 | 1.85 | 0.41 |
| 25:YA:1843:C:H2' | 25:YA:1844:C:H6 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2743:C:C1' | 55:Y9:26:ILE:HG12 | 2.51 | 0.41 |
| 25:YA:278:A:H4' | 25:YA:279:C:OP1 | 2.21 | 0.41 |
| 25:YA:2832:U:H1' | 25:YA:2834:G:C4 | 2.54 | 0.41 |
| 25:YA:306:U:H2' | 25:YA:307:G:O4' | 2.20 | 0.41 |
| 25:YA:812:C:H5'' | 25:YA:1250:G:O2' | 2.20 | 0.41 |
| 25:YA:835:A:C2 | 25:YA:836:G:C8 | 3.09 | 0.41 |
| 25:YA:923:C:H2' | 25:YA:924:C:H6 | 1.86 | 0.41 |
| 1:QA:1099:G:OP2 | 2:QB:148:TYR:OH | 2.38 | 0.41 |
| 1:QA:1179:A:H2' | 1:QA:1180:A:O4' | 2.21 | 0.41 |
| 1:QA:181:G:O2' | 1:QA:182:U:P | 2.78 | 0.41 |
| 1:QA:358:U:H2' | 1:QA:359:U:H6 | 1.84 | 0.41 |
| 1:QA:400:C:H2' | 1:QA:401:C:H6 | 1.84 | 0.41 |
| 1:QA:541:G:H2' | 1:QA:542:G:C8 | 2.55 | 0.41 |
| 1:QA:701:C:O2 | 1:QA:703:G:N1 | 2.54 | 0.41 |
| 5:QE:90:VAL:O | 5:QE:120:THR:HA | 2.21 | 0.41 |
| 6:QF:8:ILE:HD13 | 6:QF:26:ILE:HD13 | 2.02 | 0.41 |
| 8:QH:51:VAL:HG11 | 8:QH:60:ARG:HH11 | 1.86 | 0.41 |
| 13:QM:32:GLU:OE2 | 13:QM:59:TYR:OH | 2.38 | 0.41 |
| 13:QM:9:ILE:HD12 | 13:QM:9:ILE:O | 2.20 | 0.41 |
| 15:QO:3:ILE:HG13 | 15:QO:3:ILE:O | 2.20 | 0.41 |
| 53:R7:9:ARG:NH1 | 53:R7:47:ARG:HG3 | 2.35 | 0.41 |
| 25:RA:1207:C:H2' | 25:RA:1208:C:H6 | 1.86 | 0.41 |
| 25:RA:1503:U:H2' | 25:RA:1504:C:H6 | 1.84 | 0.41 |
| 25:RA:2037:G:H2' | 25:RA:2038:G:H8 | 1.85 | 0.41 |
| 25:RA:2039:C:H2' | 25:RA:2040:C:C6 | 2.56 | 0.41 |
| 25:RA:2462:U:H2' | 25:RA:2463:C:H6 | 1.86 | 0.41 |
| 25:RA:2478:A:C8 | 25:RA:2529:G:C5 | 3.09 | 0.41 |
| 25:RA:43:G:H2' | 25:RA:44:A:C8 | 2.56 | 0.41 |
| 25:RA:557:U:H2' | 25:RA:558:G:H8 | 1.86 | 0.41 |
| 25:RA:949:C:H2' | 25:RA:950:G:H8 | 1.85 | 0.41 |
| 30:RG:169:ALA:O | 30:RG:173:LEU:HG | 2.21 | 0.41 |
| 30:RG:95:ARG:O | 30:RG:99:MET:HG2 | 2.19 | 0.41 |
| 31:RH:105:LEU:HD13 | 31:RH:107:VAL:HG13 | 2.03 | 0.41 |
| 1:XA:514:C:H2' | 1:XA:515:G:C8 | 2.49 | 0.41 |
| 2:XB:20:GLU:HB2 | 2:XB:190:THR:OG1 | 2.20 | 0.41 |
| 1:XA:544:G:OP1 | 4:XD:62:GLN:HG3 | 2.20 | 0.41 |
| 10:XJ:38:ILE:HG13 | 10:XJ:71:LEU:HB3 | 2.02 | 0.41 |
| 16:XP:26:ARG:HG3 | 16:XP:27:LYS:N | 2.35 | 0.41 |
| 16:XP:6:LEU:HG | 16:XP:19:ILE:HD13 | 2.03 | 0.41 |
| 1:XA:255:G:H4' | 17:XQ:17:LYS:HB2 | 2.02 | 0.41 |
| 25:YA:1062:G:C8 | 25:YA:1088:A:C5 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:1113:U:H2' | 25:YA:1114:G:H8 | 1.85 | 0.41 |
| 25:YA:1604:C:H2' | 25:YA:1605:C:C6 | 2.55 | 0.41 |
| 25:YA:1676:A:H2' | 25:YA:1677:A:O4' | 2.20 | 0.41 |
| 25:YA:1799:G:H3' | 25:YA:1799:G:P | 2.61 | 0.41 |
| 25:YA:2525:G:H1' | 55:Y9:28:GLU:HA | 2.02 | 0.41 |
| 25:YA:2677:G:C6 | 25:YA:2731:G:C6 | 3.09 | 0.41 |
| 25:YA:38:A:H2' | 25:YA:39:C:H6 | 1.84 | 0.41 |
| 25:YA:631:A:N3 | 25:YA:2415:G:O2' | 2.45 | 0.41 |
| 25:YA:784:A:O4' | 27:YD:227:ASN:ND2 | 2.54 | 0.41 |
| 25:YA:838:C:C2 | 25:YA:941:A:C6 | 3.09 | 0.41 |
| 25:YA:924:C:H2' | 25:YA:925:C:C6 | 2.55 | 0.41 |
| 26:YB:61:G:H2' | 26:YB:62:C:C6 | 2.55 | 0.41 |
| 26:YB:78:A:H2' | 26:YB:79:C:O4' | 2.21 | 0.41 |
| 27:YD:36:PRO:HB3 | 27:YD:61:LEU:HB3 | 2.02 | 0.41 |
| 28:YE:109:LYS:HE2 | 28:YE:191:PRO:HB3 | 2.01 | 0.41 |
| 25:YA:2314:C:H5'' | 30:YG:38:VAL:HG21 | 2.03 | 0.41 |
| 31:YH:126:PRO:HB2 | 31:YH:130:ARG:O | 2.21 | 0.41 |
| 25:YA:559:G:H22 | 40:YU:49:HIS:CE1 | 2.38 | 0.41 |
| 40:YU:91:ASP:C | 40:YU:93:LYS:H | 2.24 | 0.41 |
| 43:YX:30:VAL:HG21 | 43:YX:39:ILE:HD11 | 2.02 | 0.41 |
| 44:YY:28:LYS:N | 44:YY:38:ILE:O | 2.53 | 0.41 |
| 1:QA:1022:G:H2' | 1:QA:1023:G:H8 | 1.84 | 0.41 |
| 1:QA:1351:U:H5 | 9:QI:118:LYS:NZ | 2.18 | 0.41 |
| 1:QA:227:G:H2' | 1:QA:228:A:C8 | 2.56 | 0.41 |
| 1:QA:284:G:H2' | 1:QA:285:G:H8 | 1.86 | 0.41 |
| 1:QA:519:C:H2' | 1:QA:520:A:O4' | 2.21 | 0.41 |
| 1:QA:559:A:H4' | 1:QA:560:U:H3' | 2.02 | 0.41 |
| 1:QA:64:G:H5' | 1:QA:65:U:OP1 | 2.20 | 0.41 |
| 8:QH:16:ALA:HB2 | 8:QH:24:THR:HG21 | 2.03 | 0.41 |
| 18:QR:74:ARG:HG2 | 18:QR:81:PHE:CD1 | 2.55 | 0.41 |
| 22:QV:20:G:H4' | 22:QV:21:U:OP2 | 2.19 | 0.41 |
| 22:QV:26:C:C2 | 22:QV:27:G:C8 | 3.09 | 0.41 |
| 55:R9:26:ILE:HG22 | 55:R9:33:LYS:HE3 | 2.03 | 0.41 |
| 25:RA:110:G:H2' | 25:RA:111:A:H8 | 1.84 | 0.41 |
| 25:RA:1523:U:H2' | 25:RA:1524:G:C8 | 2.56 | 0.41 |
| 25:RA:1707:G:C5 | 25:RA:1756:G:C6 | 3.08 | 0.41 |
| 25:RA:1864:U:OP1 | 25:RA:2410:G:O2' | 2.39 | 0.41 |
| 25:RA:2199:A:OP1 | 47:R1:50:ARG:NH2 | 2.34 | 0.41 |
| 25:RA:223:A:O2' | 25:RA:420:C:O2 | 2.37 | 0.41 |
| 25:RA:2740:A:H2' | 25:RA:2741:A:C8 | 2.55 | 0.41 |
| 27:RD:52:ARG:HH21 | 27:RD:53:PHE:HE2 | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:RE:35:GLN:HE21 | 28:RE:37:ARG:NH2 | 2.19 | 0.41 |
| 30:RG:129:GLY:HA2 | 30:RG:169:ALA:HB2 | 2.03 | 0.41 |
| 32:RI:68:LEU:HA | 32:RI:71:ILE:HG22 | 2.02 | 0.41 |
| 45:RZ:125:LEU:HB3 | 45:RZ:165:VAL:HG22 | 2.01 | 0.41 |
| 1:XA:1032:A:C5 | 1:XA:1032(A):G:H1' | 2.55 | 0.41 |
| 1:XA:1285:A:H1' | 1:XA:1286:A:OP2 | 2.20 | 0.41 |
| 1:XA:1384:C:H2' | 1:XA:1385:G:C8 | 2.55 | 0.41 |
| 4:QD:196:LEU:HD23 | 6:XF:16:GLN:NE2 | 2.36 | 0.41 |
| 10:XJ:51:ARG:CZ | 10:XJ:61:GLU:HB3 | 2.51 | 0.41 |
| 1:XA:265:G:H4' | 17:XQ:66:SER:HA | 2.02 | 0.41 |
| 20:XT:79:ARG:HE | 20:XT:83:ARG:HH12 | 1.69 | 0.41 |
| 20:XT:89:ARG:HD2 | 20:XT:104:LEU:HD21 | 2.02 | 0.41 |
| 25:YA:2271:G:OP1 | 46:Y0:18:ALA:HB1 | 2.20 | 0.41 |
| 48:Y2:28:LYS:HD2 | 48:Y2:53:LEU:HD11 | 2.03 | 0.41 |
| 25:YA:2756:U:C5' | 55:Y9:3:VAL:HG21 | 2.51 | 0.41 |
| 25:YA:84:A:C2 | 25:YA:103:A:C5 | 3.08 | 0.41 |
| 25:YA:1062:G:H2' | 25:YA:1063:G:H8 | 1.85 | 0.41 |
| 25:YA:1103:A:H5'' | 25:YA:1104:C:H5 | 1.86 | 0.41 |
| 25:YA:1329:U:H5'' | 25:YA:1330:C:C5 | 2.56 | 0.41 |
| 25:YA:1454:U:H5' | 37:YR:63:ARG:NH2 | 2.35 | 0.41 |
| 25:YA:2090:G:C6 | 25:YA:2230:G:C6 | 3.08 | 0.41 |
| 25:YA:2230:G:C6 | 25:YA:2231:C:C4 | 3.09 | 0.41 |
| 25:YA:236:C:H2' | 25:YA:237:C:H6 | 1.86 | 0.41 |
| 25:YA:2808:U:O2 | 25:YA:2809:A:C8 | 2.74 | 0.41 |
| 25:YA:459:U:H2' | 25:YA:460:A:C8 | 2.56 | 0.41 |
| 29:YF:160:ASN:ND2 | 29:YF:163:VAL:HG23 | 2.35 | 0.41 |
| 30:YG:111:LEU:HB3 | 30:YG:117:PHE:CZ | 2.56 | 0.41 |
| 31:YH:10:PRO:HG3 | 31:YH:69:ARG:NH1 | 2.34 | 0.41 |
| 35:YP:108:LYS:H | 35:YP:108:LYS:HD2 | 1.85 | 0.41 |
| 39:YT:111:ARG:C | 39:YT:113:LYS:N | 2.73 | 0.41 |
| 1:QA:1083:U:O2' | 1:QA:1102:A:OP2 | 2.26 | 0.41 |
| 1:QA:1129:C:O2 | 1:QA:1132:C:N4 | 2.54 | 0.41 |
| 1:QA:1362:C:HO2' | 1:QA:1362(A):C:H6 | 1.66 | 0.41 |
| 1:QA:1376:U:H2' | 1:QA:1377:A:C8 | 2.56 | 0.41 |
| 1:QA:1524:C:H2' | 1:QA:1525:G:C8 | 2.56 | 0.41 |
| 1:QA:502:G:H2' | 1:QA:503:C:O4' | 2.21 | 0.41 |
| 2:QB:21:ARG:HG3 | 2:QB:38:GLY:C | 2.41 | 0.41 |
| 4:QD:112:VAL:HG12 | 4:QD:116:GLN:OE1 | 2.21 | 0.41 |
| 10:QJ:38:ILE:HG13 | 10:QJ:38:ILE:O | 2.21 | 0.41 |
| 10:QJ:50:ILE:HG23 | 10:QJ:56:HIS:O | 2.20 | 0.41 |
| 11:QK:20:TYR:CE1 | 11:QK:83:ILE:HD12 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:R0:40:GLN:OE1 | 46:R0:44:ARG:HB2 | 2.20 | 0.41 |
| 48:R2:66:GLU:HG2 | 48:R2:69:ARG:HH21 | 1.85 | 0.41 |
| 49:R3:40:THR:HG22 | 49:R3:42:ALA:H | 1.86 | 0.41 |
| 55:R9:7:VAL:HG21 | 55:R9:23:VAL:O | 2.21 | 0.41 |
| 25:RA:1771:C:H2' | 25:RA:1772:G:H8 | 1.86 | 0.41 |
| 25:RA:48:G:N2 | 25:RA:177:G:H21 | 2.19 | 0.41 |
| 25:RA:579:G:O2' | 25:RA:2019:A:OP1 | 2.29 | 0.41 |
| 25:RA:2020:A:H4' | 40:RU:25:TRP:CZ3 | 2.55 | 0.41 |
| 25:RA:2593:U:H2' | 25:RA:2594:C:H6 | 1.86 | 0.41 |
| 25:RA:262:A:H2' | 25:RA:263:C:O4' | 2.21 | 0.41 |
| 25:RA:609:A:H2' | 25:RA:609(A):G:O4' | 2.21 | 0.41 |
| 25:RA:827:U:O2 | 25:RA:2246:G:H4' | 2.19 | 0.41 |
| 34:RO:68:GLU:HA | 34:RO:78:ARG:HB3 | 2.02 | 0.41 |
| 1:XA:1346:A:O2' | 1:XA:1347:G:H4' | 2.21 | 0.41 |
| 1:XA:1440:C:H2' | 1:XA:1441:G:O4' | 2.20 | 0.41 |
| 1:XA:186(E):C:H2' | 1:XA:186(F):C:C6 | 2.56 | 0.41 |
| 1:XA:603:U:H2' | 1:XA:604:G:C8 | 2.56 | 0.41 |
| 1:XA:827:U:H6 | 1:XA:827:U:H2' | 1.72 | 0.41 |
| 16:XP:39:TYR:HD1 | 16:XP:49:LEU:HD13 | 1.86 | 0.41 |
| 16:XP:72:ARG:HG3 | 16:XP:73:LEU:HD12 | 2.02 | 0.41 |
| 22:XW:10:G:C6 | 22:XW:27:G:C5 | 3.09 | 0.41 |
| 25:YA:1054:A:H3' | 25:YA:1055:G:H8 | 1.86 | 0.41 |
| 25:YA:1637:A:H2' | 25:YA:1638:C:C6 | 2.56 | 0.41 |
| 25:YA:2210:G:N3 | 25:YA:2210:G:H2' | 2.35 | 0.41 |
| 25:YA:2330:G:H2' | 25:YA:2331:G:O4' | 2.20 | 0.41 |
| 25:YA:2540:C:H1' | 25:YA:2741:A:C4 | 2.56 | 0.41 |
| 25:YA:588:U:O5' | 25:YA:588:U:H6 | 2.04 | 0.41 |
| 25:YA:708:C:H2' | 25:YA:709:U:C6 | 2.55 | 0.41 |
| 25:YA:862:G:H21 | 26:YB:99:A:H2 | 1.67 | 0.41 |
| 26:YB:3:C:H2' | 26:YB:4:C:H6 | 1.86 | 0.41 |
| 29:YF:32:LEU:HB3 | 29:YF:112:MET:HE1 | 2.02 | 0.41 |
| 25:YA:320:A:C2' | 29:YF:169:ASN:HD22 | 2.33 | 0.41 |
| 29:YF:60:SER:OG | 29:YF:61:GLY:N | 2.53 | 0.41 |
| 1:QA:552:U:O2 | 12:QL:31:PRO:HB3 | 2.21 | 0.41 |
| 1:QA:553:A:H2' | 1:QA:554:C:C6 | 2.56 | 0.41 |
| 1:QA:696:A:H2' | 1:QA:697:U:H6 | 1.84 | 0.41 |
| 1:QA:728:A:H2' | 1:QA:729:A:C8 | 2.56 | 0.41 |
| 2:QB:16:HIS:ND1 | 2:QB:210:SER:HA | 2.35 | 0.41 |
| 12:QL:45:PRO:HB3 | 12:QL:53:ARG:NH1 | 2.36 | 0.41 |
| 18:QR:36:ASN:HB3 | 18:QR:39:VAL:HB | 2.03 | 0.41 |
| 22:QW:14:A:C4 | 22:QW:23:G:C2 | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:99:U:H4' | 25:RA:101:G:O5' | 2.20 | 0.41 |
| 25:RA:1173:G:H4' | 25:RA:1174:A:C5 | 2.56 | 0.41 |
| 25:RA:1550:C:H2' | 25:RA:1551:C:H6 | 1.85 | 0.41 |
| 25:RA:1561:G:H2' | 25:RA:1562:A:C8 | 2.56 | 0.41 |
| 25:RA:2036:C:H2' | 25:RA:2037:G:H8 | 1.86 | 0.41 |
| 25:RA:2294:C:H2' | 25:RA:2295:C:C6 | 2.55 | 0.41 |
| 25:RA:2795:G:H3' | 25:RA:2797:U:H5'' | 2.02 | 0.41 |
| 25:RA:413:C:H2' | 25:RA:414:C:C6 | 2.56 | 0.41 |
| 25:RA:527:C:H2' | 25:RA:2779:U:H5 | 1.86 | 0.41 |
| 25:RA:646:A:H2' | 25:RA:647:G:O4' | 2.21 | 0.41 |
| 25:RA:774:A:O2' | 25:RA:775:G:O5' | 2.39 | 0.41 |
| 25:RA:820:A:H2' | 25:RA:821:A:C8 | 2.56 | 0.41 |
| 27:RD:145:VAL:HG22 | 27:RD:191:ALA:HB1 | 2.02 | 0.41 |
| 27:RD:233:HIS:NE2 | 27:RD:246:PRO:HA | 2.36 | 0.41 |
| 29:RF:110:LEU:HD11 | 29:RF:181:LEU:HG | 2.03 | 0.41 |
| 29:RF:78:ILE:HA | 29:RF:83:PHE:CD2 | 2.56 | 0.41 |
| 33:RN:22:THR:HG23 | 33:RN:62:VAL:HA | 2.03 | 0.41 |
| 41:RV:40:LEU:CD2 | 41:RV:47:VAL:HG12 | 2.51 | 0.41 |
| 1:XA:1011:G:H2' | 1:XA:1012:U:C6 | 2.55 | 0.41 |
| 1:XA:1049:U:H4' | 1:XA:1050:G:H5'' | 2.02 | 0.41 |
| 1:XA:1376:U:H2' | 1:XA:1377:A:C8 | 2.56 | 0.41 |
| 1:XA:677:U:O2 | 1:XA:777:A:O2' | 2.39 | 0.41 |
| 4:XD:111:ALA:HB2 | 4:XD:120:LEU:HD12 | 2.02 | 0.41 |
| 18:XR:81:PHE:N | 18:XR:81:PHE:CD1 | 2.89 | 0.41 |
| 22:XV:4:G:O2' | 22:XV:5:G:H8 | 2.03 | 0.41 |
| 22:XW:41:C:H2' | 22:XW:42:C:H6 | 1.85 | 0.41 |
| 47:Y1:51:VAL:HG11 | 47:Y1:74:VAL:HG21 | 2.03 | 0.41 |
| 25:YA:1007:C:H5'' | 33:YN:35:ARG:NH1 | 2.36 | 0.41 |
| 25:YA:1112:G:H2' | 25:YA:1113:U:C6 | 2.55 | 0.41 |
| 25:YA:1297:C:H2' | 25:YA:1298:C:C6 | 2.55 | 0.41 |
| 25:YA:1475:G:H2' | 25:YA:1476:C:H6 | 1.86 | 0.41 |
| 25:YA:2315:G:OP1 | 30:YG:36:LYS:NZ | 2.39 | 0.41 |
| 25:YA:2747:G:N1 | 25:YA:2755:C:H4' | 2.36 | 0.41 |
| 25:YA:2755:C:H6 | 25:YA:2755:C:C5' | 2.34 | 0.41 |
| 25:YA:573:G:O2' | 25:YA:574:C:H3' | 2.21 | 0.41 |
| 25:YA:2073:C:C5' | 27:YD:229:VAL:HG22 | 2.50 | 0.41 |
| 30:YG:63:ILE:HG22 | 30:YG:143:GLU:HB2 | 2.03 | 0.41 |
| 37:YR:104:ARG:HD2 | 37:YR:107:ASP:OD2 | 2.19 | 0.41 |
| 39:YT:34:VAL:HG12 | 39:YT:36:GLU:HG2 | 2.02 | 0.41 |
| 45:YZ:112:ARG:HG3 | 45:YZ:113:ALA:H | 1.85 | 0.41 |
| 1:QA:1043:C:H2' | 1:QA:1044:A:C8 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1429:C:H2' | 1:QA:1430:C:C6 | 2.56 | 0.41 |
| 1:QA:191(F):U:H2' | 1:QA:191:G:H8 | 1.86 | 0.41 |
| 1:QA:55:A:C2 | 32:YI:89:TYR:CD2 | 3.09 | 0.41 |
| 1:QA:645:C:H2' | 1:QA:646:U:C6 | 2.56 | 0.41 |
| 3:QC:34:LEU:HD12 | 14:QN:25:VAL:HG21 | 2.02 | 0.41 |
| 4:QD:19:LEU:HB2 | 4:QD:67:ILE:HG12 | 2.03 | 0.41 |
| 8:QH:97:VAL:HG21 | 8:QH:128:GLY:HA2 | 2.03 | 0.41 |
| 9:QI:32:ASP:OD1 | 9:QI:33:PHE:N | 2.54 | 0.41 |
| 11:QK:20:TYR:CD1 | 11:QK:83:ILE:HB | 2.56 | 0.41 |
| 16:QP:23:ASP:OD1 | 16:QP:24:ALA:N | 2.54 | 0.41 |
| 17:QQ:95:TYR:HD1 | 17:QQ:98:LEU:HD12 | 1.86 | 0.41 |
| 22:QW:15:G:N2 | 22:QW:60:A:N7 | 2.69 | 0.41 |
| 13:QM:3:ARG:HB2 | 50:R4:34:GLU:HB3 | 2.02 | 0.41 |
| 54:R8:32:LEU:O | 54:R8:36:LYS:HE3 | 2.21 | 0.41 |
| 25:RA:1201:C:H2' | 25:RA:1202:C:C6 | 2.56 | 0.41 |
| 25:RA:1482:U:H3 | 25:RA:1512:G:H1 | 1.69 | 0.41 |
| 25:RA:1535:U:H2' | 25:RA:1536:A:N7 | 2.36 | 0.41 |
| 25:RA:2625:G:H2' | 25:RA:2626:C:C6 | 2.55 | 0.41 |
| 25:RA:690:G:H4' | 27:RD:218:ARG:HH22 | 1.85 | 0.41 |
| 28:RE:63:LEU:HD12 | 28:RE:65:GLY:N | 2.36 | 0.41 |
| 30:RG:23:PHE:CE2 | 30:RG:168:GLU:HG2 | 2.56 | 0.41 |
| 41:RV:38:LEU:HD12 | 41:RV:57:VAL:HG13 | 2.03 | 0.41 |
| 1:XA:1368:G:H5'' | 9:XI:112:LYS:HB3 | 2.03 | 0.41 |
| 1:XA:323:U:H2' | 1:XA:324:G:O4' | 2.19 | 0.41 |
| 1:XA:57:G:N2 | 1:XA:388:G:O6 | 2.41 | 0.41 |
| 1:XA:59:A:H5'' | 1:XA:60:A:H5'' | 2.03 | 0.41 |
| 1:XA:875:C:O2' | 8:XH:14:ARG:HD2 | 2.20 | 0.41 |
| 2:XB:71:VAL:HG23 | 2:XB:93:VAL:HB | 2.03 | 0.41 |
| 6:XF:8:ILE:HG22 | 6:XF:10:LEU:HD12 | 2.03 | 0.41 |
| 12:XL:66:VAL:HG21 | 12:XL:98:TYR:CE2 | 2.56 | 0.41 |
| 17:XQ:95:TYR:HD1 | 17:XQ:98:LEU:HD12 | 1.86 | 0.41 |
| 18:XR:47:THR:O | 18:XR:83:GLU:N | 2.54 | 0.41 |
| 22:XW:52:C:O2 | 22:XW:65:G:N2 | 2.54 | 0.41 |
| 25:YA:125:G:H5' | 53:Y7:19:ARG:HD3 | 2.03 | 0.41 |
| 55:Y9:32:HIS:HB3 | 55:Y9:34:GLN:HE21 | 1.86 | 0.41 |
| 25:YA:1266:G:N7 | 42:YW:15:ARG:HD2 | 2.36 | 0.41 |
| 25:YA:1316:U:H2' | 25:YA:1317:A:H8 | 1.80 | 0.41 |
| 25:YA:1595:G:H2' | 25:YA:1596:A:C8 | 2.56 | 0.41 |
| 25:YA:1958:C:H2' | 25:YA:1959:G:H8 | 1.84 | 0.41 |
| 25:YA:2273:A:H2' | 25:YA:2274:A:C8 | 2.56 | 0.41 |
| 25:YA:2293:C:H2' | 25:YA:2294:C:H6 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:272:G:H2' | 25:YA:273:G:C8 | 2.55 | 0.41 |
| 25:YA:2743:C:C4' | 55:Y9:26:ILE:H | 2.33 | 0.41 |
| 25:YA:39:C:H2' | 25:YA:40:C:C6 | 2.56 | 0.41 |
| 25:YA:609(A):G:H2' | 25:YA:610:C:H6 | 1.86 | 0.41 |
| 26:YB:60:C:H2' | 26:YB:61:G:H8 | 1.86 | 0.41 |
| 28:YE:29:GLY:HA2 | 28:YE:180:ASN:HB3 | 2.02 | 0.41 |
| 30:YG:114:ILE:HB | 30:YG:117:PHE:HB2 | 2.03 | 0.41 |
| 35:YP:37:GLY:O | 35:YP:41:ARG:HG2 | 2.21 | 0.41 |
| 36:YQ:139:GLU:N | 36:YQ:139:GLU:OE1 | 2.54 | 0.41 |
| 36:YQ:19:GLY:O | 36:YQ:98:LYS:HD3 | 2.20 | 0.41 |
| 45:YZ:54:HIS:ND1 | 45:YZ:101:PRO:HG3 | 2.36 | 0.41 |
| 45:YZ:58:VAL:O | 45:YZ:59:LEU:HB2 | 2.21 | 0.41 |
| 1:QA:955:U:H1' | 1:QA:1227:A:H61 | 1.85 | 0.41 |
| 1:QA:763:G:H2' | 1:QA:764:C:C6 | 2.55 | 0.41 |
| 3:QC:150:LYS:HG3 | 3:QC:169:ALA:HB2 | 2.03 | 0.41 |
| 8:QH:12:ARG:NH1 | 8:QH:26:VAL:HA | 2.36 | 0.41 |
| 6:QF:50:TYR:CE1 | 18:QR:77:GLY:HA2 | 2.56 | 0.41 |
| 19:QS:50:ALA:HA | 19:QS:58:VAL:O | 2.20 | 0.41 |
| 22:QW:10:G:N2 | 22:QW:27:G:H1' | 2.36 | 0.41 |
| 48:R2:17:SER:OG | 48:R2:20:GLU:HG2 | 2.20 | 0.41 |
| 25:RA:1108:U:H2' | 25:RA:1109:C:C2 | 2.56 | 0.41 |
| 25:RA:839:U:O2' | 25:RA:1191:G:N3 | 2.53 | 0.41 |
| 25:RA:1210:A:H5' | 25:RA:1211:U:H2' | 2.03 | 0.41 |
| 25:RA:1278:A:H5" | 37:RR:36:THR:HG22 | 2.03 | 0.41 |
| 25:RA:1291:C:C2 | 25:RA:1292:U:C5 | 3.09 | 0.41 |
| 25:RA:1346:G:C6 | 25:RA:1601:G:C6 | 3.09 | 0.41 |
| 25:RA:2271:G:H2' | 25:RA:2272:U:C6 | 2.56 | 0.41 |
| 25:RA:2721:A:C4 | 25:RA:2722:G:C8 | 3.09 | 0.41 |
| 25:RA:2848:G:O2' | 25:RA:2867:G:N2 | 2.53 | 0.41 |
| 1:XA:253:U:H2' | 1:XA:254:G:C8 | 2.56 | 0.41 |
| 1:XA:812:C:H1' | 1:XA:813:U:OP2 | 2.21 | 0.41 |
| 9:XI:9:ARG:HG2 | 9:XI:14:VAL:HG22 | 2.02 | 0.41 |
| 9:XI:6:GLY:HA3 | 9:XI:84:ALA:HB2 | 2.02 | 0.41 |
| 10:XJ:6:ILE:HG22 | 10:XJ:98:ILE:HG13 | 2.03 | 0.41 |
| 16:XP:82:GLN:HG2 | 16:XP:84:ALA:H | 1.86 | 0.41 |
| 25:YA:94:G:N3 | 48:Y2:47:ASN:ND2 | 2.69 | 0.41 |
| 25:YA:1321:A:C4 | 25:YA:1322:A:C8 | 3.09 | 0.41 |
| 25:YA:1530:G:H2' | 25:YA:1531:C:C6 | 2.57 | 0.41 |
| 25:YA:1794:U:H2' | 25:YA:1795:C:C6 | 2.56 | 0.41 |
| 25:YA:2108:C:H2' | 25:YA:2109:U:C6 | 2.56 | 0.41 |
| 25:YA:2408:U:H2' | 25:YA:2409:G:H8 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:2417:C:C2 | 25:YA:2418:A:C8 | 3.08 | 0.41 |
| 25:YA:2706:G:O2' | 37:YR:64:ARG:HD3 | 2.20 | 0.41 |
| 25:YA:2867:G:O2' | 25:YA:2868:A:H8 | 1.84 | 0.41 |
| 25:YA:392:C:H5'' | 25:YA:409:C:H5'' | 2.03 | 0.41 |
| 25:YA:593:G:H2' | 25:YA:594:U:H6 | 1.84 | 0.41 |
| 25:YA:792:G:N3 | 25:YA:2072:G:O2' | 2.34 | 0.41 |
| 30:YG:40:ASN:HD22 | 30:YG:41:GLN:N | 2.17 | 0.41 |
| 32:YI:49:ALA:HA | 32:YI:52:ARG:HG2 | 2.03 | 0.41 |
| 39:YT:6:LEU:O | 39:YT:10:VAL:HG23 | 2.21 | 0.41 |
| 1:QA:1219:U:C2 | 1:QA:1220:G:C8 | 3.10 | 0.40 |
| 1:QA:1418:A:N3 | 25:RA:1959:G:H1' | 2.36 | 0.40 |
| 1:QA:579:G:H5' | 1:QA:728:A:H1' | 2.03 | 0.40 |
| 3:QC:130:VAL:O | 3:QC:134:ILE:HG12 | 2.22 | 0.40 |
| 22:QW:60:A:H2' | 22:QW:61:U:O4' | 2.21 | 0.40 |
| 46:R0:53:MET:HA | 46:R0:58:THR:O | 2.21 | 0.40 |
| 47:R1:83:GLU:HG2 | 47:R1:85:LEU:H | 1.86 | 0.40 |
| 25:RA:2755:C:H42 | 55:R9:1:MET:H2 | 1.68 | 0.40 |
| 25:RA:1429:G:H2' | 25:RA:1430:C:C6 | 2.56 | 0.40 |
| 25:RA:1660:C:H2' | 25:RA:1661:G:H8 | 1.86 | 0.40 |
| 25:RA:2114:A:N6 | 25:RA:2119:A:H62 | 2.19 | 0.40 |
| 25:RA:2704:C:H2' | 25:RA:2705:A:O4' | 2.21 | 0.40 |
| 25:RA:363:G:H2' | 25:RA:363(A):A:H8 | 1.85 | 0.40 |
| 25:RA:900:A:N3 | 25:RA:900:A:H2' | 2.36 | 0.40 |
| 28:RE:35:GLN:HE21 | 28:RE:37:ARG:CZ | 2.34 | 0.40 |
| 32:RI:21:VAL:HG22 | 32:RI:22:LYS:H | 1.86 | 0.40 |
| 41:RV:49:THR:HB | 41:RV:50:PRO:HD2 | 2.03 | 0.40 |
| 44:RY:13:VAL:HB | 44:RY:72:VAL:HG13 | 2.03 | 0.40 |
| 1:XA:579:G:O2' | 15:XO:54:ARG:NE | 2.53 | 0.40 |
| 1:XA:881:G:H2' | 1:XA:882:C:O4' | 2.21 | 0.40 |
| 2:XB:189:ASP:HB3 | 2:XB:203:GLY:O | 2.20 | 0.40 |
| 4:XD:68:TYR:OH | 4:XD:196:LEU:HD11 | 2.21 | 0.40 |
| 1:XA:1148:U:O3' | 9:XI:14:VAL:HG11 | 2.21 | 0.40 |
| 9:XI:77:ILE:O | 9:XI:81:ILE:HG12 | 2.21 | 0.40 |
| 10:XJ:45:ARG:HB3 | 10:XJ:65:LEU:HB3 | 2.02 | 0.40 |
| 10:XJ:50:ILE:CD1 | 10:XJ:60:ARG:HE | 2.33 | 0.40 |
| 11:XK:84:VAL:CG1 | 11:XK:95:ILE:HD11 | 2.51 | 0.40 |
| 13:XM:12:ASN:O | 13:XM:13:LYS:HB2 | 2.21 | 0.40 |
| 22:XW:41:C:H2' | 22:XW:42:C:C6 | 2.56 | 0.40 |
| 30:YG:3:LEU:HD21 | 50:Y4:25:TYR:HD2 | 1.86 | 0.40 |
| 25:YA:1005:C:H5' | 25:YA:1012:U:H1' | 2.03 | 0.40 |
| 25:YA:116:C:O2' | 25:YA:126:A:N3 | 2.47 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1422:G:H4' | 25:YA:1493:C:OP1 | 2.21 | 0.40 |
| 25:YA:1668:A:N3 | 25:YA:1670:C:C4 | 2.89 | 0.40 |
| 25:YA:1907:G:H2' | 25:YA:1908:C:H6 | 1.85 | 0.40 |
| 25:YA:2025:C:H2' | 25:YA:2026:C:H6 | 1.86 | 0.40 |
| 25:YA:2047:U:H2' | 25:YA:2048:G:C8 | 2.54 | 0.40 |
| 25:YA:242:G:H4' | 25:YA:243:U:O5' | 2.21 | 0.40 |
| 25:YA:2747:G:N1 | 25:YA:2755:C:P | 2.94 | 0.40 |
| 25:YA:2893:G:H5'' | 25:YA:2894:G:OP1 | 2.20 | 0.40 |
| 25:YA:313:C:H2' | 25:YA:314:A:H8 | 1.85 | 0.40 |
| 25:YA:680:G:H2' | 25:YA:681:G:C8 | 2.56 | 0.40 |
| 25:YA:720:C:H2' | 25:YA:721:C:C6 | 2.54 | 0.40 |
| 28:YE:103:ASP:OD2 | 28:YE:201:THR:HA | 2.20 | 0.40 |
| 29:YF:181:LEU:HD11 | 29:YF:186:ILE:HD11 | 2.04 | 0.40 |
| 33:YN:67:LEU:O | 33:YN:88:GLU:HB2 | 2.21 | 0.40 |
| 29:YF:34:TRP:CE2 | 35:YP:8:PRO:HG3 | 2.56 | 0.40 |
| 25:YA:2847:U:OP1 | 39:YT:98:LYS:HD3 | 2.21 | 0.40 |
| 25:YA:567:A:N6 | 41:YV:78:LYS:HD3 | 2.36 | 0.40 |
| 45:YZ:48:PHE:HE1 | 45:YZ:71:VAL:HG11 | 1.84 | 0.40 |
| 1:QA:452:A:O2' | 16:QP:72:ARG:HD2 | 2.20 | 0.40 |
| 1:QA:500:G:H2' | 1:QA:501:C:C6 | 2.56 | 0.40 |
| 1:QA:557:G:H2' | 1:QA:558:G:C8 | 2.56 | 0.40 |
| 1:QA:992:U:H1' | 1:QA:993:G:OP2 | 2.22 | 0.40 |
| 4:QD:57:ARG:HB3 | 4:QD:206:PHE:HD1 | 1.85 | 0.40 |
| 22:QW:52:C:O2 | 22:QW:65:G:N2 | 2.54 | 0.40 |
| 25:RA:1173:G:H21 | 25:RA:1175:U:H5 | 1.69 | 0.40 |
| 25:RA:1291:C:H2' | 25:RA:1292:U:C6 | 2.56 | 0.40 |
| 25:RA:1469:A:H2' | 25:RA:1470:G:O4' | 2.20 | 0.40 |
| 25:RA:1419:A:C8 | 25:RA:1579:A:N6 | 2.89 | 0.40 |
| 25:RA:2314:C:H2' | 25:RA:2315:G:C8 | 2.56 | 0.40 |
| 25:RA:2327:A:H2' | 25:RA:2328:A:C8 | 2.57 | 0.40 |
| 25:RA:2437:U:H2' | 25:RA:2438:U:C6 | 2.57 | 0.40 |
| 25:RA:2521:C:O2' | 25:RA:2564:A:N3 | 2.50 | 0.40 |
| 25:RA:270(P):C:H2' | 25:RA:270(Q):C:H6 | 1.86 | 0.40 |
| 25:RA:436:C:H2' | 25:RA:438:G:C8 | 2.56 | 0.40 |
| 25:RA:554:U:H2' | 25:RA:556:G:N7 | 2.37 | 0.40 |
| 26:RB:73:A:N3 | 26:RB:73:A:H2' | 2.36 | 0.40 |
| 30:RG:60:LEU:O | 30:RG:64:THR:HG22 | 2.22 | 0.40 |
| 39:RT:19:LEU:HD22 | 39:RT:86:ILE:HG22 | 2.01 | 0.40 |
| 45:RZ:145:GLU:CG | 45:RZ:146:ILE:H | 2.33 | 0.40 |
| 1:XA:1421:G:C6 | 1:XA:1480:G:C6 | 3.09 | 0.40 |
| 1:XA:35:G:H2' | 1:XA:36:C:C6 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:374:A:C6 | 1:XA:375:U:C4 | 3.09 | 0.40 |
| 1:XA:679:C:H2' | 1:XA:680:C:H6 | 1.87 | 0.40 |
| 1:XA:738:C:H2' | 1:XA:739:C:C6 | 2.55 | 0.40 |
| 2:XB:155:LEU:O | 2:XB:157:ARG:N | 2.48 | 0.40 |
| 7:XG:116:ALA:O | 7:XG:120:ILE:HG12 | 2.21 | 0.40 |
| 1:XA:235:C:H1' | 17:XQ:61:GLU:OE1 | 2.21 | 0.40 |
| 22:XW:23:G:C2 | 22:XW:24:C:C5 | 3.09 | 0.40 |
| 49:Y3:7:LYS:HA | 49:Y3:33:GLN:O | 2.21 | 0.40 |
| 25:YA:978:G:O4' | 25:YA:1001:A:H2 | 2.04 | 0.40 |
| 25:YA:171:G:H2' | 25:YA:172:C:C6 | 2.56 | 0.40 |
| 25:YA:1751:C:H2' | 25:YA:1752:C:C6 | 2.57 | 0.40 |
| 25:YA:1862:G:H2' | 25:YA:1863:G:H8 | 1.86 | 0.40 |
| 25:YA:1266:G:O2' | 25:YA:2012:G:O6 | 2.27 | 0.40 |
| 25:YA:2186:G:H2' | 25:YA:2187:G:C8 | 2.56 | 0.40 |
| 25:YA:2521:C:C2 | 25:YA:2545:G:N2 | 2.89 | 0.40 |
| 25:YA:2685:G:P | 39:YT:51:ARG:HH22 | 2.44 | 0.40 |
| 25:YA:2712:U:H5'' | 25:YA:2714:G:H5' | 2.03 | 0.40 |
| 25:YA:2795:G:H3' | 25:YA:2797:U:H5'' | 2.02 | 0.40 |
| 25:YA:38:A:N3 | 29:YF:48:THR:OG1 | 2.53 | 0.40 |
| 25:YA:416:C:H2' | 25:YA:417:C:C6 | 2.56 | 0.40 |
| 25:YA:872:A:N6 | 25:YA:906:G:C6 | 2.89 | 0.40 |
| 27:YD:77:ALA:HB2 | 27:YD:97:TYR:CD1 | 2.57 | 0.40 |
| 28:YE:63:LEU:HD12 | 28:YE:65:GLY:N | 2.37 | 0.40 |
| 36:YQ:81:VAL:HG23 | 36:YQ:82:ARG:N | 2.34 | 0.40 |
| 1:QA:608:A:C2 | 1:QA:609:A:H1' | 2.57 | 0.40 |
| 4:QD:64:LEU:HB2 | 4:QD:198:VAL:HG11 | 2.03 | 0.40 |
| 17:QQ:18:THR:OG1 | 17:QQ:69:LYS:NZ | 2.35 | 0.40 |
| 25:RA:1009:A:N3 | 25:RA:1153:C:O2' | 2.44 | 0.40 |
| 25:RA:1314:C:H5'' | 25:RA:1610:A:H61 | 1.87 | 0.40 |
| 25:RA:1478:G:H1' | 25:RA:1557:C:O2' | 2.22 | 0.40 |
| 25:RA:1671:U:N3 | 25:RA:1674:G:OP2 | 2.50 | 0.40 |
| 25:RA:1891:G:H2' | 25:RA:1892:C:C6 | 2.56 | 0.40 |
| 25:RA:2025:C:H2' | 25:RA:2026:C:H6 | 1.86 | 0.40 |
| 25:RA:2112:G:O6 | 25:RA:2169:A:N6 | 2.54 | 0.40 |
| 25:RA:2466:C:C4 | 25:RA:2467:C:N4 | 2.89 | 0.40 |
| 25:RA:2677:G:H2' | 25:RA:2678:C:C6 | 2.55 | 0.40 |
| 25:RA:2787:C:O2' | 25:RA:2810:A:O2' | 2.37 | 0.40 |
| 25:RA:2846:G:H2' | 25:RA:2847:U:H6 | 1.87 | 0.40 |
| 25:RA:315:G:H2' | 25:RA:316:C:C6 | 2.55 | 0.40 |
| 25:RA:541:C:H2' | 25:RA:542:C:C6 | 2.56 | 0.40 |
| 27:RD:31:LYS:HG3 | 27:RD:32:SER:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:40:GLN:HE22 | 29:RF:182:ASN:ND2 | 2.19 | 0.40 |
| 29:RF:64:ILE:HG23 | 29:RF:65:TRP:N | 2.36 | 0.40 |
| 34:RO:107:ARG:HB2 | 34:RO:115:VAL:HG11 | 2.02 | 0.40 |
| 37:RR:91:GLN:O | 37:RR:91:GLN:HG2 | 2.21 | 0.40 |
| 37:RR:98:LEU:O | 37:RR:113:LEU:N | 2.43 | 0.40 |
| 38:RS:61:ASN:O | 38:RS:64:GLU:N | 2.54 | 0.40 |
| 39:RT:34:VAL:HG12 | 39:RT:36:GLU:HG2 | 2.03 | 0.40 |
| 25:RA:1754:C:P | 39:RT:96:ARG:HH12 | 2.44 | 0.40 |
| 1:XA:1144:G:H21 | 1:XA:1146:A:H62 | 1.70 | 0.40 |
| 1:XA:682:G:H2' | 1:XA:683:G:H8 | 1.86 | 0.40 |
| 1:XA:963:G:H21 | 10:XJ:55:LYS:CD | 2.34 | 0.40 |
| 1:XA:997:U:H2' | 1:XA:998:G:C8 | 2.55 | 0.40 |
| 9:XI:10:ARG:HH21 | 9:XI:107:ARG:HE | 1.69 | 0.40 |
| 9:XI:114:TYR:HB2 | 10:XJ:60:ARG:HH11 | 1.86 | 0.40 |
| 22:XW:33:C:H5' | 22:XW:34:U:OP2 | 2.22 | 0.40 |
| 22:XW:15:G:N2 | 22:XW:60:A:N7 | 2.70 | 0.40 |
| 50:Y4:47:GLN:O | 50:Y4:48:ARG:C | 2.60 | 0.40 |
| 35:YP:62:LEU:HD22 | 54:Y8:27:THR:HA | 2.02 | 0.40 |
| 54:Y8:29:LYS:HA | 54:Y8:36:LYS:NZ | 2.37 | 0.40 |
| 25:YA:1298:C:H2' | 25:YA:1299:G:O4' | 2.22 | 0.40 |
| 25:YA:1406:U:H3' | 25:YA:1407:C:H6 | 1.86 | 0.40 |
| 25:YA:185:U:H2' | 25:YA:186:G:H8 | 1.85 | 0.40 |
| 25:YA:1930:G:H2' | 25:YA:1968:G:N1 | 2.36 | 0.40 |
| 25:YA:2051:A:H5' | 25:YA:2578:G:O4' | 2.21 | 0.40 |
| 25:YA:2208:U:H2' | 25:YA:2209:C:C6 | 2.56 | 0.40 |
| 25:YA:2408:U:H2' | 25:YA:2409:G:C8 | 2.56 | 0.40 |
| 25:YA:247:G:H4' | 25:YA:386:G:C4 | 2.57 | 0.40 |
| 25:YA:2566:A:H4' | 25:YA:2567:G:O5' | 2.21 | 0.40 |
| 25:YA:270(U):C:H2' | 25:YA:270(V):G:C8 | 2.56 | 0.40 |
| 25:YA:465:G:H21 | 25:YA:684:G:H1' | 1.85 | 0.40 |
| 25:YA:520:G:H2' | 25:YA:521:G:C8 | 2.56 | 0.40 |
| 25:YA:536:A:OP1 | 40:YU:53:ARG:NH1 | 2.54 | 0.40 |
| 25:YA:564:C:H2' | 25:YA:565:C:H6 | 1.87 | 0.40 |
| 25:YA:970:C:H2' | 25:YA:971:C:C6 | 2.56 | 0.40 |
| 31:YH:146:ALA:HA | 55:Y9:20:HIS:HB3 | 2.03 | 0.40 |
| 25:YA:1187:G:H5'' | 41:YV:81:TYR:CE1 | 2.56 | 0.40 |
| 1:QA:1126:U:H1' | 1:QA:1280:A:C5 | 2.56 | 0.40 |
| 1:QA:1150:U:H2' | 1:QA:1151:A:C8 | 2.56 | 0.40 |
| 1:QA:1264:C:H2' | 1:QA:1265:G:H8 | 1.85 | 0.40 |
| 1:QA:1319:A:C8 | 1:QA:1323:G:C5 | 3.09 | 0.40 |
| 1:QA:604:G:H2' | 1:QA:605:U:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:578:C:O2' | 1:QA:728:A:N3 | 2.52 | 0.40 |
| 1:QA:939:G:H2' | 1:QA:940:C:H6 | 1.86 | 0.40 |
| 11:QK:93:GLN:OE1 | 11:QK:96:ARG:NH2 | 2.48 | 0.40 |
| 22:QV:35:C:HO2' | 22:QV:36:A:P | 2.44 | 0.40 |
| 25:RA:117:G:H4' | 53:R7:18:PHE:CE2 | 2.56 | 0.40 |
| 25:RA:1292:U:C2 | 25:RA:1293:C:C5 | 3.09 | 0.40 |
| 25:RA:1375:C:H2' | 25:RA:1376:C:C6 | 2.57 | 0.40 |
| 25:RA:1407:C:O2 | 25:RA:1407:C:H2' | 2.22 | 0.40 |
| 25:RA:1694:C:H4' | 25:RA:1695:G:O5' | 2.21 | 0.40 |
| 25:RA:1800:C:H3' | 27:RD:147:LEU:HD22 | 2.04 | 0.40 |
| 25:RA:2009:G:C6 | 25:RA:2010:G:N7 | 2.90 | 0.40 |
| 25:RA:2416:C:C2 | 25:RA:2417:C:C5 | 3.10 | 0.40 |
| 25:RA:2530:A:N7 | 31:RH:172:LYS:NZ | 2.60 | 0.40 |
| 25:RA:1669:A:O3' | 25:RA:2549:G:H5' | 2.22 | 0.40 |
| 25:RA:2771:C:H2' | 25:RA:2772:C:H6 | 1.85 | 0.40 |
| 25:RA:2820:A:H4' | 37:RR:3:HIS:ND1 | 2.37 | 0.40 |
| 25:RA:493:G:H4' | 42:RW:8:ARG:HB2 | 2.04 | 0.40 |
| 25:RA:918:A:C5 | 25:RA:919:G:H1' | 2.56 | 0.40 |
| 31:RH:9:ILE:HA | 31:RH:10:PRO:HD3 | 1.90 | 0.40 |
| 31:RH:149:ARG:HG2 | 31:RH:149:ARG:O | 2.21 | 0.40 |
| 33:RN:22:THR:HA | 33:RN:61:ARG:O | 2.22 | 0.40 |
| 34:RO:64:ARG:HG2 | 34:RO:79:PHE:CD2 | 2.56 | 0.40 |
| 36:RQ:73:PRO:HA | 36:RQ:93:TYR:CD1 | 2.56 | 0.40 |
| 38:RS:10:ARG:HG2 | 38:RS:13:ARG:NH2 | 2.35 | 0.40 |
| 39:RT:30:VAL:HB | 39:RT:86:ILE:HG13 | 2.03 | 0.40 |
| 42:RW:13:SER:HB3 | 42:RW:16:LYS:HD2 | 2.03 | 0.40 |
| 1:XA:1004:A:H8 | 1:XA:1036:G:H22 | 1.68 | 0.40 |
| 1:XA:1010:G:H2' | 1:XA:1011:G:C8 | 2.57 | 0.40 |
| 1:XA:392:G:H2' | 1:XA:393:A:C8 | 2.57 | 0.40 |
| 1:XA:405:U:H3' | 1:XA:406:G:H5' | 2.04 | 0.40 |
| 1:XA:913:A:H4' | 1:XA:914:A:O5' | 2.21 | 0.40 |
| 2:XB:16:HIS:HD2 | 2:XB:210:SER:CA | 2.34 | 0.40 |
| 4:XD:10:ARG:HG3 | 4:XD:40:PRO:CG | 2.51 | 0.40 |
| 11:XK:21:ILE:HB | 11:XK:84:VAL:HG12 | 2.02 | 0.40 |
| 22:XW:20:G:H3' | 22:XW:21:U:H5 | 1.87 | 0.40 |
| 46:Y0:68:GLU:HG3 | 46:Y0:80:HIS:HB2 | 2.04 | 0.40 |
| 25:YA:1085:A:H2' | 25:YA:1086:A:C4 | 2.57 | 0.40 |
| 25:YA:1993:U:H4' | 28:YE:128:SER:OG | 2.22 | 0.40 |
| 25:YA:2250:G:C4 | 36:YQ:82:ARG:HG3 | 2.57 | 0.40 |
| 25:YA:2712:U:HO2' | 25:YA:2712(A):A:P | 2.44 | 0.40 |
| 25:YA:2773:C:H2' | 25:YA:2774:C:H6 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:37:C:H2' | 25:YA:38:A:H8 | 1.87 | 0.40 |
| 25:YA:529:A:H8 | 25:YA:530:G:C6 | 2.40 | 0.40 |
| 26:YB:73:A:H2' | 26:YB:73:A:N3 | 2.36 | 0.40 |
| 27:YD:34:VAL:HG13 | 27:YD:34:VAL:O | 2.22 | 0.40 |
| 30:YG:81:LYS:HB3 | 30:YG:82:LEU:H | 1.69 | 0.40 |
| 36:YQ:77:LYS:NZ | 36:YQ:84:GLY:O | 2.41 | 0.40 |
| 37:YR:13:HIS:CE1 | 37:YR:16:HIS:HB2 | 2.57 | 0.40 |
| 39:YT:39:ARG:HG2 | 39:YT:40:THR:H | 1.86 | 0.40 |
| 40:YU:11:ARG:O | 40:YU:15:LYS:HG2 | 2.22 | 0.40 |
| 40:YU:92:ARG:C | 40:YU:94:ASN:N | 2.72 | 0.40 |
| 40:YU:92:ARG:HH21 | 41:YV:10:LYS:HB3 | 1.86 | 0.40 |
| 1:QA:1013:G:N2 | 1:QA:1015:A:H3' | 2.36 | 0.40 |
| 1:QA:1072:G:H2' | 1:QA:1073:U:C6 | 2.56 | 0.40 |
| 1:QA:1325:C:H4' | 21:QU:17:THR:HG21 | 2.02 | 0.40 |
| 1:QA:229:U:H2' | 1:QA:230:G:C8 | 2.56 | 0.40 |
| 1:QA:235:C:H2' | 1:QA:236:G:C8 | 2.53 | 0.40 |
| 3:QC:129:ALA:HB3 | 3:QC:132:ARG:HB3 | 2.03 | 0.40 |
| 3:QC:134:ILE:HG23 | 3:QC:151:VAL:HB | 2.04 | 0.40 |
| 3:QC:30:ARG:HD2 | 14:QN:38:GLY:HA3 | 2.03 | 0.40 |
| 4:QD:13:ARG:HH12 | 4:QD:36:ARG:CZ | 2.35 | 0.40 |
| 9:QI:97:LYS:HB3 | 9:QI:98:PRO:HD3 | 2.03 | 0.40 |
| 1:QA:975:A:N1 | 10:QJ:48:THR:HB | 2.36 | 0.40 |
| 16:QP:82:GLN:HG2 | 16:QP:84:ALA:H | 1.86 | 0.40 |
| 20:QT:30:LYS:HZ2 | 20:QT:80:ARG:NH1 | 2.20 | 0.40 |
| 22:QW:41:C:H2' | 22:QW:42:C:H6 | 1.87 | 0.40 |
| 52:R6:9:LEU:HA | 52:R6:54:ILE:HB | 2.03 | 0.40 |
| 25:RA:108:U:H4' | 25:RA:347:A:H2 | 1.86 | 0.40 |
| 25:RA:1416:G:H2' | 25:RA:1417:C:H6 | 1.85 | 0.40 |
| 25:RA:1802:A:H2' | 25:RA:1803:A:H8 | 1.85 | 0.40 |
| 25:RA:1826:G:H2' | 25:RA:1827:C:C6 | 2.56 | 0.40 |
| 25:RA:1910:G:H2' | 25:RA:1911:U:O4' | 2.22 | 0.40 |
| 25:RA:25:U:H5' | 42:RW:79:GLY:HA2 | 2.03 | 0.40 |
| 25:RA:270(U):C:C2 | 25:RA:270(V):G:C8 | 3.10 | 0.40 |
| 25:RA:2752:C:O2 | 25:RA:2752:C:H2' | 2.21 | 0.40 |
| 28:RE:117:MET:HA | 28:RE:122:PHE:H | 1.85 | 0.40 |
| 31:RH:4:ILE:H | 31:RH:4:ILE:HD12 | 1.85 | 0.40 |
| 33:RN:21:LYS:HG2 | 33:RN:26:LEU:HD13 | 2.03 | 0.40 |
| 35:RP:107:LYS:O | 35:RP:109:GLY:N | 2.55 | 0.40 |
| 45:RZ:6:LYS:HD2 | 45:RZ:8:TYR:CZ | 2.57 | 0.40 |
| 1:XA:1095:U:H2' | 1:XA:1096:C:C6 | 2.55 | 0.40 |
| 1:XA:1101:A:N6 | 2:XB:176:GLU:OE2 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:1499:A:C1' | 1:XA:1520:G:H5' | 2.52 | 0.40 |
| 1:XA:595:G:H21 | 1:XA:596:C:H42 | 1.70 | 0.40 |
| 1:XA:704:A:H2' | 1:XA:704:A:N3 | 2.36 | 0.40 |
| 1:XA:704:A:H8 | 1:XA:704:A:OP2 | 2.04 | 0.40 |
| 16:XP:53:VAL:O | 16:XP:57:ARG:HG2 | 2.22 | 0.40 |
| 13:XM:3:ARG:NH2 | 50:Y4:34:GLU:OE2 | 2.54 | 0.40 |
| 50:Y4:37:SER:O | 50:Y4:43:TYR:HD2 | 2.04 | 0.40 |
| 25:YA:2744:G:N7 | 55:Y9:1:MET:HE3 | 2.37 | 0.40 |
| 55:Y9:31:LYS:HD3 | 55:Y9:32:HIS:CE1 | 2.57 | 0.40 |
| 55:Y9:2:LYS:HB2 | 55:Y9:32:HIS:HA | 2.03 | 0.40 |
| 25:YA:1662:C:H2' | 25:YA:1663:C:C6 | 2.56 | 0.40 |
| 25:YA:1794:U:H2' | 25:YA:1795:C:H6 | 1.86 | 0.40 |
| 25:YA:2078:C:H2' | 25:YA:2079:U:C6 | 2.56 | 0.40 |
| 25:YA:2181:G:H2' | 25:YA:2182:G:C8 | 2.56 | 0.40 |
| 25:YA:546:C:OP1 | 25:YA:547:A:N6 | 2.55 | 0.40 |
| 25:YA:565:C:H2' | 25:YA:566:U:C6 | 2.57 | 0.40 |
| 25:YA:598:G:H2' | 25:YA:599:G:O4' | 2.22 | 0.40 |
| 25:YA:601:C:O2' | 25:YA:605:C:H5'' | 2.21 | 0.40 |
| 25:YA:719:C:H2' | 25:YA:720:C:H6 | 1.87 | 0.40 |
| 25:YA:874:G:H2' | 25:YA:875:G:C8 | 2.57 | 0.40 |
| 25:YA:910:A:C5 | 36:YQ:13:GLN:HG3 | 2.55 | 0.40 |
| 26:YB:46:A:C5 | 26:YB:47:C:C5 | 3.09 | 0.40 |
| 28:YE:82:ARG:O | 28:YE:83:ASP:HB2 | 2.21 | 0.40 |
| 30:YG:41:GLN:HE21 | 30:YG:153:ARG:HB3 | 1.86 | 0.40 |
| 32:YI:11:ASN:O | 32:YI:12:LEU:HD12 | 2.22 | 0.40 |
| 25:YA:1278:A:OP1 | 37:YR:36:THR:HG22 | 2.21 | 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) |
|------------------|-------------------------|--------------------------|-------------------|
| 42:RW:63:ASP:OD1 | 44:YY:92:ASN:ND2[3_555] | 2.18 | 0.02 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | QB | 233/256 (91%) | 202 (87%) | 29 (12%) | 2 (1%) | 17 | 54 |
| 2 | XB | 234/256 (91%) | 202 (86%) | 31 (13%) | 1 (0%) | 34 | 69 |
| 3 | QC | 203/239 (85%) | 188 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | XC | 203/239 (85%) | 190 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | QD | 206/209 (99%) | 189 (92%) | 17 (8%) | 0 | 100 | 100 |
| 4 | XD | 206/209 (99%) | 190 (92%) | 16 (8%) | 0 | 100 | 100 |
| 5 | QE | 149/162 (92%) | 141 (95%) | 7 (5%) | 1 (1%) | 22 | 59 |
| 5 | XE | 149/162 (92%) | 140 (94%) | 8 (5%) | 1 (1%) | 22 | 59 |
| 6 | QF | 99/101 (98%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | XF | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | QG | 153/156 (98%) | 147 (96%) | 6 (4%) | 0 | 100 | 100 |
| 7 | XG | 153/156 (98%) | 148 (97%) | 5 (3%) | 0 | 100 | 100 |
| 8 | QH | 135/138 (98%) | 129 (96%) | 6 (4%) | 0 | 100 | 100 |
| 8 | XH | 135/138 (98%) | 126 (93%) | 9 (7%) | 0 | 100 | 100 |
| 9 | QI | 125/128 (98%) | 112 (90%) | 13 (10%) | 0 | 100 | 100 |
| 9 | XI | 124/128 (97%) | 112 (90%) | 12 (10%) | 0 | 100 | 100 |
| 10 | QJ | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 10 | XJ | 94/105 (90%) | 84 (89%) | 10 (11%) | 0 | 100 | 100 |
| 11 | QK | 117/129 (91%) | 109 (93%) | 8 (7%) | 0 | 100 | 100 |
| 11 | XK | 114/129 (88%) | 108 (95%) | 6 (5%) | 0 | 100 | 100 |
| 12 | QL | 123/132 (93%) | 105 (85%) | 18 (15%) | 0 | 100 | 100 |
| 12 | XL | 120/132 (91%) | 97 (81%) | 22 (18%) | 1 (1%) | 19 | 56 |
| 13 | QM | 118/126 (94%) | 96 (81%) | 21 (18%) | 1 (1%) | 19 | 56 |
| 13 | XM | 117/126 (93%) | 94 (80%) | 22 (19%) | 1 (1%) | 17 | 54 |
| 14 | QN | 58/61 (95%) | 54 (93%) | 3 (5%) | 1 (2%) | 9 | 42 |
| 14 | XN | 58/61 (95%) | 54 (93%) | 3 (5%) | 1 (2%) | 9 | 42 |
| 15 | QO | 86/89 (97%) | 81 (94%) | 5 (6%) | 0 | 100 | 100 |
| 15 | XO | 85/89 (96%) | 84 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | QP | 82/88 (93%) | 79 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | XP | 82/88 (93%) | 78 (95%) | 4 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 17 | QQ | 98/105 (93%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | XQ | 98/105 (93%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | QR | 68/88 (77%) | 64 (94%) | 4 (6%) | 0 | 100 | 100 |
| 18 | XR | 68/88 (77%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 19 | QS | 81/93 (87%) | 70 (86%) | 11 (14%) | 0 | 100 | 100 |
| 19 | XS | 82/93 (88%) | 70 (85%) | 11 (13%) | 1 (1%) | 13 | 49 |
| 20 | QT | 97/106 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 20 | XT | 97/106 (92%) | 87 (90%) | 10 (10%) | 0 | 100 | 100 |
| 21 | QU | 23/27 (85%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 21 | XU | 23/27 (85%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 27 | RD | 270/276 (98%) | 235 (87%) | 33 (12%) | 2 (1%) | 22 | 59 |
| 27 | YD | 270/276 (98%) | 239 (88%) | 29 (11%) | 2 (1%) | 22 | 59 |
| 28 | RE | 203/206 (98%) | 163 (80%) | 37 (18%) | 3 (2%) | 10 | 44 |
| 28 | YE | 203/206 (98%) | 158 (78%) | 42 (21%) | 3 (2%) | 10 | 44 |
| 29 | RF | 200/210 (95%) | 183 (92%) | 17 (8%) | 0 | 100 | 100 |
| 29 | YF | 200/210 (95%) | 185 (92%) | 13 (6%) | 2 (1%) | 15 | 51 |
| 30 | RG | 179/182 (98%) | 149 (83%) | 29 (16%) | 1 (1%) | 25 | 62 |
| 30 | YG | 179/182 (98%) | 148 (83%) | 29 (16%) | 2 (1%) | 14 | 50 |
| 31 | RH | 172/180 (96%) | 141 (82%) | 28 (16%) | 3 (2%) | 9 | 42 |
| 31 | YH | 172/180 (96%) | 137 (80%) | 32 (19%) | 3 (2%) | 9 | 42 |
| 32 | RI | 144/148 (97%) | 119 (83%) | 22 (15%) | 3 (2%) | 7 | 38 |
| 32 | YI | 144/148 (97%) | 117 (81%) | 24 (17%) | 3 (2%) | 7 | 38 |
| 33 | RN | 136/140 (97%) | 117 (86%) | 17 (12%) | 2 (2%) | 10 | 44 |
| 33 | YN | 136/140 (97%) | 117 (86%) | 18 (13%) | 1 (1%) | 22 | 59 |
| 34 | RO | 120/122 (98%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 34 | YO | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 35 | RP | 148/150 (99%) | 114 (77%) | 33 (22%) | 1 (1%) | 22 | 59 |
| 35 | YP | 145/150 (97%) | 112 (77%) | 32 (22%) | 1 (1%) | 22 | 59 |
| 36 | RQ | 139/141 (99%) | 114 (82%) | 24 (17%) | 1 (1%) | 22 | 59 |
| 36 | YQ | 139/141 (99%) | 116 (84%) | 21 (15%) | 2 (1%) | 11 | 45 |
| 37 | RR | 115/118 (98%) | 102 (89%) | 13 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 37 | YR | 115/118 (98%) | 103 (90%) | 11 (10%) | 1 (1%) | 17 | 54 |
| 38 | RS | 109/112 (97%) | 86 (79%) | 23 (21%) | 0 | 100 | 100 |
| 38 | YS | 109/112 (97%) | 87 (80%) | 22 (20%) | 0 | 100 | 100 |
| 39 | RT | 135/146 (92%) | 115 (85%) | 18 (13%) | 2 (2%) | 10 | 44 |
| 39 | YT | 135/146 (92%) | 115 (85%) | 18 (13%) | 2 (2%) | 10 | 44 |
| 40 | RU | 115/118 (98%) | 109 (95%) | 5 (4%) | 1 (1%) | 17 | 54 |
| 40 | YU | 115/118 (98%) | 109 (95%) | 5 (4%) | 1 (1%) | 17 | 54 |
| 41 | RV | 99/101 (98%) | 86 (87%) | 12 (12%) | 1 (1%) | 15 | 51 |
| 41 | YV | 99/101 (98%) | 86 (87%) | 13 (13%) | 0 | 100 | 100 |
| 42 | RW | 111/113 (98%) | 103 (93%) | 8 (7%) | 0 | 100 | 100 |
| 42 | YW | 111/113 (98%) | 98 (88%) | 13 (12%) | 0 | 100 | 100 |
| 43 | RX | 90/96 (94%) | 87 (97%) | 3 (3%) | 0 | 100 | 100 |
| 43 | YX | 90/96 (94%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 44 | RY | 105/110 (96%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 44 | YY | 105/110 (96%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 45 | RZ | 181/206 (88%) | 144 (80%) | 33 (18%) | 4 (2%) | 6 | 37 |
| 45 | YZ | 181/206 (88%) | 142 (78%) | 36 (20%) | 3 (2%) | 9 | 42 |
| 46 | R0 | 79/85 (93%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 46 | Y0 | 73/85 (86%) | 69 (94%) | 4 (6%) | 0 | 100 | 100 |
| 47 | R1 | 95/98 (97%) | 85 (90%) | 9 (10%) | 1 (1%) | 14 | 50 |
| 47 | Y1 | 91/98 (93%) | 77 (85%) | 13 (14%) | 1 (1%) | 14 | 50 |
| 48 | R2 | 67/72 (93%) | 62 (92%) | 4 (6%) | 1 (2%) | 10 | 44 |
| 48 | Y2 | 67/72 (93%) | 61 (91%) | 5 (8%) | 1 (2%) | 10 | 44 |
| 49 | R3 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 49 | Y3 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 50 | R4 | 67/71 (94%) | 53 (79%) | 13 (19%) | 1 (2%) | 10 | 44 |
| 50 | Y4 | 67/71 (94%) | 53 (79%) | 13 (19%) | 1 (2%) | 10 | 44 |
| 51 | R5 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 51 | Y5 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 52 | R6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 52 | Y6 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 53 | R7 | 45/49 (92%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | Y7 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | R8 | 62/65 (95%) | 46 (74%) | 14 (23%) | 2 (3%) | 4 | 31 |
| 54 | Y8 | 62/65 (95%) | 47 (76%) | 13 (21%) | 2 (3%) | 4 | 31 |
| 55 | R9 | 35/37 (95%) | 25 (71%) | 10 (29%) | 0 | 100 | 100 |
| 55 | Y9 | 35/37 (95%) | 18 (51%) | 15 (43%) | 2 (6%) | 1 | 19 |
| All | All | 11452/12128 (94%) | 10130 (88%) | 1249 (11%) | 73 (1%) | 25 | 62 |

All (73) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | RE | 18 | ASP |
| 31 | RH | 87 | LEU |
| 32 | RI | 15 | VAL |
| 35 | RP | 108 | LYS |
| 39 | RT | 124 | ASP |
| 40 | RU | 92 | ARG |
| 45 | RZ | 53 | ILE |
| 45 | RZ | 180 | VAL |
| 54 | R8 | 29 | LYS |
| 54 | R8 | 30 | ARG |
| 28 | YE | 18 | ASP |
| 31 | YH | 87 | LEU |
| 32 | YI | 15 | VAL |
| 35 | YP | 108 | LYS |
| 39 | YT | 124 | ASP |
| 45 | YZ | 53 | ILE |
| 45 | YZ | 180 | VAL |
| 54 | Y8 | 29 | LYS |
| 54 | Y8 | 30 | ARG |
| 2 | QB | 208 | ILE |
| 14 | QN | 17 | LYS |
| 27 | RD | 34 | VAL |
| 27 | RD | 243 | GLY |
| 33 | RN | 22 | THR |
| 39 | RT | 123 | GLN |
| 50 | R4 | 47 | GLN |
| 14 | XN | 17 | LYS |
| 33 | YN | 22 | THR |
| 39 | YT | 123 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | YU | 92 | ARG |
| 50 | Y4 | 47 | GLN |
| 55 | Y9 | 30 | PRO |
| 13 | QM | 14 | ARG |
| 32 | RI | 11 | ASN |
| 48 | R2 | 70 | GLN |
| 27 | YD | 34 | VAL |
| 27 | YD | 243 | GLY |
| 32 | YI | 11 | ASN |
| 37 | YR | 4 | LEU |
| 45 | YZ | 178 | GLU |
| 48 | Y2 | 70 | GLN |
| 28 | RE | 83 | ASP |
| 30 | RG | 81 | LYS |
| 31 | RH | 86 | GLU |
| 41 | RV | 44 | LYS |
| 45 | RZ | 178 | GLU |
| 12 | XL | 105 | TYR |
| 19 | XS | 27 | GLU |
| 28 | YE | 63 | LEU |
| 28 | YE | 83 | ASP |
| 30 | YG | 81 | LYS |
| 31 | YH | 86 | GLU |
| 55 | Y9 | 28 | GLU |
| 47 | R1 | 54 | ALA |
| 13 | XM | 14 | ARG |
| 29 | YF | 67 | GLN |
| 29 | YF | 129 | PHE |
| 28 | RE | 145 | LYS |
| 33 | RN | 96 | GLU |
| 36 | RQ | 78 | PRO |
| 30 | YG | 82 | LEU |
| 31 | YH | 12 | PRO |
| 36 | YQ | 22 | LYS |
| 36 | YQ | 78 | PRO |
| 47 | Y1 | 54 | ALA |
| 31 | RH | 12 | PRO |
| 2 | XB | 208 | ILE |
| 2 | QB | 232 | PRO |
| 5 | QE | 74 | GLY |
| 32 | RI | 16 | GLY |
| 5 | XE | 74 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | YI | 16 | GLY |
| 45 | RZ | 166 | SER |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | QB | 203/220 (92%) | 202 (100%) | 1 (0%) | 88 | 94 |
| 2 | XB | 204/220 (93%) | 201 (98%) | 3 (2%) | 65 | 81 |
| 3 | QC | 159/188 (85%) | 159 (100%) | 0 | 100 | 100 |
| 3 | XC | 159/188 (85%) | 159 (100%) | 0 | 100 | 100 |
| 4 | QD | 180/181 (99%) | 178 (99%) | 2 (1%) | 73 | 85 |
| 4 | XD | 180/181 (99%) | 178 (99%) | 2 (1%) | 73 | 85 |
| 5 | QE | 116/123 (94%) | 116 (100%) | 0 | 100 | 100 |
| 5 | XE | 116/123 (94%) | 116 (100%) | 0 | 100 | 100 |
| 6 | QF | 90/90 (100%) | 88 (98%) | 2 (2%) | 52 | 72 |
| 6 | XF | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 7 | QG | 126/127 (99%) | 126 (100%) | 0 | 100 | 100 |
| 7 | XG | 126/127 (99%) | 126 (100%) | 0 | 100 | 100 |
| 8 | QH | 118/119 (99%) | 117 (99%) | 1 (1%) | 81 | 89 |
| 8 | XH | 118/119 (99%) | 117 (99%) | 1 (1%) | 81 | 89 |
| 9 | QI | 98/99 (99%) | 96 (98%) | 2 (2%) | 55 | 74 |
| 9 | XI | 97/99 (98%) | 97 (100%) | 0 | 100 | 100 |
| 10 | QJ | 89/92 (97%) | 89 (100%) | 0 | 100 | 100 |
| 10 | XJ | 86/92 (94%) | 86 (100%) | 0 | 100 | 100 |
| 11 | QK | 90/99 (91%) | 90 (100%) | 0 | 100 | 100 |
| 11 | XK | 88/99 (89%) | 88 (100%) | 0 | 100 | 100 |
| 12 | QL | 104/109 (95%) | 104 (100%) | 0 | 100 | 100 |
| 12 | XL | 103/109 (94%) | 103 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 13 | QM | 96/101 (95%) | 96 (100%) | 0 | 100 | 100 |
| 13 | XM | 95/101 (94%) | 95 (100%) | 0 | 100 | 100 |
| 14 | QN | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 74 |
| 14 | XN | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 74 |
| 15 | QO | 79/80 (99%) | 79 (100%) | 0 | 100 | 100 |
| 15 | XO | 79/80 (99%) | 79 (100%) | 0 | 100 | 100 |
| 16 | QP | 72/74 (97%) | 72 (100%) | 0 | 100 | 100 |
| 16 | XP | 72/74 (97%) | 72 (100%) | 0 | 100 | 100 |
| 17 | QQ | 95/97 (98%) | 94 (99%) | 1 (1%) | 73 | 85 |
| 17 | XQ | 95/97 (98%) | 94 (99%) | 1 (1%) | 73 | 85 |
| 18 | QR | 61/77 (79%) | 61 (100%) | 0 | 100 | 100 |
| 18 | XR | 61/77 (79%) | 61 (100%) | 0 | 100 | 100 |
| 19 | QS | 72/80 (90%) | 71 (99%) | 1 (1%) | 67 | 82 |
| 19 | XS | 73/80 (91%) | 73 (100%) | 0 | 100 | 100 |
| 20 | QT | 76/82 (93%) | 75 (99%) | 1 (1%) | 69 | 83 |
| 20 | XT | 76/82 (93%) | 75 (99%) | 1 (1%) | 69 | 83 |
| 21 | QU | 20/22 (91%) | 20 (100%) | 0 | 100 | 100 |
| 21 | XU | 20/22 (91%) | 20 (100%) | 0 | 100 | 100 |
| 27 | RD | 214/218 (98%) | 213 (100%) | 1 (0%) | 88 | 94 |
| 27 | YD | 214/218 (98%) | 213 (100%) | 1 (0%) | 88 | 94 |
| 28 | RE | 165/166 (99%) | 165 (100%) | 0 | 100 | 100 |
| 28 | YE | 165/166 (99%) | 165 (100%) | 0 | 100 | 100 |
| 29 | RF | 161/166 (97%) | 160 (99%) | 1 (1%) | 86 | 93 |
| 29 | YF | 161/166 (97%) | 160 (99%) | 1 (1%) | 86 | 93 |
| 30 | RG | 155/156 (99%) | 154 (99%) | 1 (1%) | 86 | 93 |
| 30 | YG | 155/156 (99%) | 154 (99%) | 1 (1%) | 86 | 93 |
| 31 | RH | 145/148 (98%) | 142 (98%) | 3 (2%) | 53 | 73 |
| 31 | YH | 145/148 (98%) | 142 (98%) | 3 (2%) | 53 | 73 |
| 32 | RI | 122/124 (98%) | 122 (100%) | 0 | 100 | 100 |
| 32 | YI | 122/124 (98%) | 122 (100%) | 0 | 100 | 100 |
| 33 | RN | 117/119 (98%) | 116 (99%) | 1 (1%) | 78 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 33 | YN | 117/119 (98%) | 116 (99%) | 1 (1%) | 78 | 88 |
| 34 | RO | 100/100 (100%) | 99 (99%) | 1 (1%) | 76 | 86 |
| 34 | YO | 100/100 (100%) | 99 (99%) | 1 (1%) | 76 | 86 |
| 35 | RP | 116/116 (100%) | 116 (100%) | 0 | 100 | 100 |
| 35 | YP | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 36 | RQ | 111/111 (100%) | 111 (100%) | 0 | 100 | 100 |
| 36 | YQ | 111/111 (100%) | 111 (100%) | 0 | 100 | 100 |
| 37 | RR | 100/101 (99%) | 100 (100%) | 0 | 100 | 100 |
| 37 | YR | 100/101 (99%) | 100 (100%) | 0 | 100 | 100 |
| 38 | RS | 87/88 (99%) | 86 (99%) | 1 (1%) | 73 | 85 |
| 38 | YS | 87/88 (99%) | 86 (99%) | 1 (1%) | 73 | 85 |
| 39 | RT | 120/127 (94%) | 120 (100%) | 0 | 100 | 100 |
| 39 | YT | 120/127 (94%) | 120 (100%) | 0 | 100 | 100 |
| 40 | RU | 93/94 (99%) | 92 (99%) | 1 (1%) | 73 | 85 |
| 40 | YU | 93/94 (99%) | 92 (99%) | 1 (1%) | 73 | 85 |
| 41 | RV | 82/82 (100%) | 82 (100%) | 0 | 100 | 100 |
| 41 | YV | 82/82 (100%) | 82 (100%) | 0 | 100 | 100 |
| 42 | RW | 92/92 (100%) | 90 (98%) | 2 (2%) | 52 | 72 |
| 42 | YW | 92/92 (100%) | 90 (98%) | 2 (2%) | 52 | 72 |
| 43 | RX | 74/78 (95%) | 74 (100%) | 0 | 100 | 100 |
| 43 | YX | 74/78 (95%) | 74 (100%) | 0 | 100 | 100 |
| 44 | RY | 88/91 (97%) | 88 (100%) | 0 | 100 | 100 |
| 44 | YY | 88/91 (97%) | 88 (100%) | 0 | 100 | 100 |
| 45 | RZ | 162/179 (90%) | 161 (99%) | 1 (1%) | 86 | 93 |
| 45 | YZ | 162/179 (90%) | 161 (99%) | 1 (1%) | 86 | 93 |
| 46 | R0 | 65/67 (97%) | 65 (100%) | 0 | 100 | 100 |
| 46 | Y0 | 61/67 (91%) | 60 (98%) | 1 (2%) | 62 | 79 |
| 47 | R1 | 82/83 (99%) | 82 (100%) | 0 | 100 | 100 |
| 47 | Y1 | 78/83 (94%) | 78 (100%) | 0 | 100 | 100 |
| 48 | R2 | 64/67 (96%) | 64 (100%) | 0 | 100 | 100 |
| 48 | Y2 | 64/67 (96%) | 64 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 49 | R3 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 49 | Y3 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 50 | R4 | 62/63 (98%) | 61 (98%) | 1 (2%) | 62 | 79 |
| 50 | Y4 | 62/63 (98%) | 60 (97%) | 2 (3%) | 39 | 64 |
| 51 | R5 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 51 | Y5 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 52 | R6 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 52 | Y6 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 53 | R7 | 40/42 (95%) | 40 (100%) | 0 | 100 | 100 |
| 53 | Y7 | 41/42 (98%) | 41 (100%) | 0 | 100 | 100 |
| 54 | R8 | 54/55 (98%) | 54 (100%) | 0 | 100 | 100 |
| 54 | Y8 | 54/55 (98%) | 54 (100%) | 0 | 100 | 100 |
| 55 | R9 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 55 | Y9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 66 |
| All | All | 9687/10066 (96%) | 9635 (100%) | 52 (0%) | 88 | 94 |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | QB | 30 | ARG |
| 4 | QD | 103 | ASN |
| 4 | QD | 131 | ARG |
| 6 | QF | 71 | ARG |
| 6 | QF | 80 | ARG |
| 8 | QH | 91 | ARG |
| 9 | QI | 10 | ARG |
| 9 | QI | 111 | ARG |
| 14 | QN | 45 | ARG |
| 17 | QQ | 91 | ARG |
| 19 | QS | 41 | VAL |
| 20 | QT | 86 | ARG |
| 27 | RD | 273 | ARG |
| 29 | RF | 38 | ARG |
| 30 | RG | 40 | ASN |
| 31 | RH | 23 | ARG |
| 31 | RH | 69 | ARG |
| 31 | RH | 152 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 33 | RN | 115 | ARG |
| 34 | RO | 97 | ARG |
| 38 | RS | 3 | ARG |
| 40 | RU | 94 | ASN |
| 42 | RW | 15 | ARG |
| 42 | RW | 40 | ASN |
| 45 | RZ | 34 | ASN |
| 50 | R4 | 61 | ARG |
| 2 | XB | 30 | ARG |
| 2 | XB | 64 | ARG |
| 2 | XB | 144 | ARG |
| 4 | XD | 103 | ASN |
| 4 | XD | 131 | ARG |
| 8 | XH | 91 | ARG |
| 14 | XN | 45 | ARG |
| 17 | XQ | 91 | ARG |
| 20 | XT | 86 | ARG |
| 27 | YD | 273 | ARG |
| 29 | YF | 38 | ARG |
| 30 | YG | 40 | ASN |
| 31 | YH | 23 | ARG |
| 31 | YH | 69 | ARG |
| 31 | YH | 152 | ARG |
| 33 | YN | 115 | ARG |
| 34 | YO | 97 | ARG |
| 38 | YS | 3 | ARG |
| 40 | YU | 94 | ASN |
| 42 | YW | 15 | ARG |
| 42 | YW | 40 | ASN |
| 45 | YZ | 34 | ASN |
| 46 | Y0 | 55 | ARG |
| 50 | Y4 | 56 | VAL |
| 50 | Y4 | 61 | ARG |
| 55 | Y9 | 27 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | QC | 108 | ASN |
| 4 | QD | 119 | GLN |
| 9 | QI | 3 | GLN |
| 9 | QI | 73 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | QJ | 84 | GLN |
| 29 | RF | 40 | GLN |
| 30 | RG | 40 | ASN |
| 37 | RR | 71 | GLN |
| 39 | RT | 58 | ASN |
| 42 | RW | 111 | HIS |
| 43 | RX | 41 | ASN |
| 52 | R6 | 29 | ASN |
| 2 | XB | 16 | HIS |
| 29 | YF | 40 | GLN |
| 31 | YH | 74 | ASN |
| 42 | YW | 111 | HIS |
| 44 | YY | 6 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | QA | 1498/1508 (99%) | 252 (16%) | 34 (2%) |
| 1 | XA | 1499/1508 (99%) | 272 (18%) | 37 (2%) |
| 22 | QV | 76/77 (98%) | 17 (22%) | 3 (3%) |
| 22 | QW | 75/77 (97%) | 31 (41%) | 2 (2%) |
| 22 | XV | 76/77 (98%) | 18 (23%) | 3 (3%) |
| 22 | XW | 75/77 (97%) | 32 (42%) | 2 (2%) |
| 23 | QX | 7/25 (28%) | 0 | 0 |
| 23 | XX | 9/25 (36%) | 3 (33%) | 0 |
| 24 | QY | 16/17 (94%) | 2 (12%) | 0 |
| 24 | XY | 16/17 (94%) | 2 (12%) | 0 |
| 25 | RA | 2879/2915 (98%) | 599 (20%) | 47 (1%) |
| 25 | YA | 2880/2915 (98%) | 570 (19%) | 48 (1%) |
| 26 | RB | 119/122 (97%) | 17 (14%) | 1 (0%) |
| 26 | YB | 119/122 (97%) | 19 (15%) | 1 (0%) |
| All | All | 9344/9482 (98%) | 1834 (19%) | 178 (1%) |

All (1834) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 6 | G |
| 1 | QA | 9 | G |
| 1 | QA | 32 | A |
| 1 | QA | 39 | G |
| 1 | QA | 48 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 51 | A |
| 1 | QA | 64 | G |
| 1 | QA | 65 | U |
| 1 | QA | 66 | G |
| 1 | QA | 76 | G |
| 1 | QA | 79 | G |
| 1 | QA | 80 | G |
| 1 | QA | 101 | A |
| 1 | QA | 108 | G |
| 1 | QA | 116 | A |
| 1 | QA | 120 | A |
| 1 | QA | 121 | C |
| 1 | QA | 129(A) | G |
| 1 | QA | 144 | G |
| 1 | QA | 146 | G |
| 1 | QA | 147 | G |
| 1 | QA | 163 | C |
| 1 | QA | 169 | C |
| 1 | QA | 173 | U |
| 1 | QA | 174 | C |
| 1 | QA | 182 | U |
| 1 | QA | 190 | G |
| 1 | QA | 195 | A |
| 1 | QA | 197 | A |
| 1 | QA | 209 | U |
| 1 | QA | 210 | U |
| 1 | QA | 216 | G |
| 1 | QA | 220 | G |
| 1 | QA | 244 | U |
| 1 | QA | 245 | C |
| 1 | QA | 247 | G |
| 1 | QA | 250 | A |
| 1 | QA | 251 | G |
| 1 | QA | 267 | C |
| 1 | QA | 270 | A |
| 1 | QA | 281 | G |
| 1 | QA | 289 | G |
| 1 | QA | 306 | G |
| 1 | QA | 321 | A |
| 1 | QA | 328 | C |
| 1 | QA | 329 | A |
| 1 | QA | 332 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 344 | A |
| 1 | QA | 346 | G |
| 1 | QA | 347 | G |
| 1 | QA | 351 | G |
| 1 | QA | 352 | C |
| 1 | QA | 353 | A |
| 1 | QA | 354 | G |
| 1 | QA | 367 | U |
| 1 | QA | 372 | C |
| 1 | QA | 373 | A |
| 1 | QA | 390 | C |
| 1 | QA | 397 | A |
| 1 | QA | 398 | C |
| 1 | QA | 406 | G |
| 1 | QA | 411 | A |
| 1 | QA | 412 | A |
| 1 | QA | 413 | G |
| 1 | QA | 421 | U |
| 1 | QA | 422 | C |
| 1 | QA | 423 | G |
| 1 | QA | 424 | G |
| 1 | QA | 428 | G |
| 1 | QA | 429 | U |
| 1 | QA | 448 | A |
| 1 | QA | 451 | A |
| 1 | QA | 466 | C |
| 1 | QA | 467 | G |
| 1 | QA | 482 | A |
| 1 | QA | 485 | G |
| 1 | QA | 486 | U |
| 1 | QA | 496 | A |
| 1 | QA | 497 | U |
| 1 | QA | 505 | G |
| 1 | QA | 509 | A |
| 1 | QA | 510 | A |
| 1 | QA | 511 | C |
| 1 | QA | 518 | C |
| 1 | QA | 521 | G |
| 1 | QA | 527 | G |
| 1 | QA | 532 | A |
| 1 | QA | 533 | A |
| 1 | QA | 534 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 545 | C |
| 1 | QA | 547 | A |
| 1 | QA | 559 | A |
| 1 | QA | 562 | C |
| 1 | QA | 564 | C |
| 1 | QA | 568 | G |
| 1 | QA | 572 | A |
| 1 | QA | 573 | A |
| 1 | QA | 576 | G |
| 1 | QA | 577 | G |
| 1 | QA | 596 | C |
| 1 | QA | 618 | C |
| 1 | QA | 630 | G |
| 1 | QA | 631 | G |
| 1 | QA | 633 | G |
| 1 | QA | 653 | A |
| 1 | QA | 665 | A |
| 1 | QA | 666 | G |
| 1 | QA | 686 | U |
| 1 | QA | 688 | G |
| 1 | QA | 701 | C |
| 1 | QA | 702 | A |
| 1 | QA | 703 | G |
| 1 | QA | 704 | A |
| 1 | QA | 723 | U |
| 1 | QA | 731 | G |
| 1 | QA | 748 | C |
| 1 | QA | 754 | C |
| 1 | QA | 755 | G |
| 1 | QA | 777 | A |
| 1 | QA | 792 | A |
| 1 | QA | 793 | U |
| 1 | QA | 794 | A |
| 1 | QA | 802 | A |
| 1 | QA | 813 | U |
| 1 | QA | 817 | C |
| 1 | QA | 819 | A |
| 1 | QA | 821 | G |
| 1 | QA | 828 | A |
| 1 | QA | 841 | U |
| 1 | QA | 842 | C |
| 1 | QA | 843 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 848 | C |
| 1 | QA | 859 | A |
| 1 | QA | 871 | U |
| 1 | QA | 872 | A |
| 1 | QA | 902 | G |
| 1 | QA | 914 | A |
| 1 | QA | 927 | G |
| 1 | QA | 934 | C |
| 1 | QA | 935 | A |
| 1 | QA | 960 | U |
| 1 | QA | 968 | A |
| 1 | QA | 969 | A |
| 1 | QA | 971 | G |
| 1 | QA | 972 | C |
| 1 | QA | 974 | A |
| 1 | QA | 975 | A |
| 1 | QA | 976 | G |
| 1 | QA | 977 | A |
| 1 | QA | 991 | U |
| 1 | QA | 992 | U |
| 1 | QA | 993 | G |
| 1 | QA | 994 | A |
| 1 | QA | 1001 | G |
| 1 | QA | 1004 | A |
| 1 | QA | 1009 | G |
| 1 | QA | 1024 | G |
| 1 | QA | 1025 | U |
| 1 | QA | 1028 | C |
| 1 | QA | 1029 | G |
| 1 | QA | 1031 | G |
| 1 | QA | 1032(A) | G |
| 1 | QA | 1054 | C |
| 1 | QA | 1055 | A |
| 1 | QA | 1064 | G |
| 1 | QA | 1065 | U |
| 1 | QA | 1066 | C |
| 1 | QA | 1081 | G |
| 1 | QA | 1094 | G |
| 1 | QA | 1095 | U |
| 1 | QA | 1100 | C |
| 1 | QA | 1101 | A |
| 1 | QA | 1108 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | QA | 1124 | G |
| 1 | QA | 1125 | U |
| 1 | QA | 1126 | U |
| 1 | QA | 1130 | A |
| 1 | QA | 1131 | G |
| 1 | QA | 1136 | U |
| 1 | QA | 1137 | C |
| 1 | QA | 1138 | G |
| 1 | QA | 1139 | G |
| 1 | QA | 1146 | A |
| 1 | QA | 1157 | A |
| 1 | QA | 1158 | C |
| 1 | QA | 1159 | U |
| 1 | QA | 1160 | G |
| 1 | QA | 1171 | G |
| 1 | QA | 1181 | G |
| 1 | QA | 1183 | A |
| 1 | QA | 1184 | G |
| 1 | QA | 1196 | U |
| 1 | QA | 1200 | C |
| 1 | QA | 1201 | A |
| 1 | QA | 1202 | G |
| 1 | QA | 1212 | U |
| 1 | QA | 1213 | A |
| 1 | QA | 1224 | G |
| 1 | QA | 1238 | A |
| 1 | QA | 1240 | U |
| 1 | QA | 1241 | G |
| 1 | QA | 1256 | A |
| 1 | QA | 1257 | U |
| 1 | QA | 1258 | G |
| 1 | QA | 1260 | C |
| 1 | QA | 1270 | C |
| 1 | QA | 1280 | A |
| 1 | QA | 1281 | U |
| 1 | QA | 1286 | A |
| 1 | QA | 1287 | A |
| 1 | QA | 1290 | G |
| 1 | QA | 1297 | C |
| 1 | QA | 1298 | C |
| 1 | QA | 1299 | A |
| 1 | QA | 1300 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | QA | 1302 | U |
| 1 | QA | 1303 | C |
| 1 | QA | 1305 | G |
| 1 | QA | 1320 | C |
| 1 | QA | 1321 | C |
| 1 | QA | 1322 | C |
| 1 | QA | 1323 | G |
| 1 | QA | 1331 | G |
| 1 | QA | 1335 | C |
| 1 | QA | 1336 | C |
| 1 | QA | 1337 | G |
| 1 | QA | 1338 | G |
| 1 | QA | 1347 | G |
| 1 | QA | 1348 | U |
| 1 | QA | 1362(A) | C |
| 1 | QA | 1397 | C |
| 1 | QA | 1398 | A |
| 1 | QA | 1406 | U |
| 1 | QA | 1419 | G |
| 1 | QA | 1442 | G |
| 1 | QA | 1446 | A |
| 1 | QA | 1447 | G |
| 1 | QA | 1452 | C |
| 1 | QA | 1453 | G |
| 1 | QA | 1487 | G |
| 1 | QA | 1492 | A |
| 1 | QA | 1494 | G |
| 1 | QA | 1499 | A |
| 1 | QA | 1503 | A |
| 1 | QA | 1504 | G |
| 1 | QA | 1506 | U |
| 1 | QA | 1507 | A |
| 1 | QA | 1517 | G |
| 1 | QA | 1519 | A |
| 1 | QA | 1520 | G |
| 1 | QA | 1529 | G |
| 1 | QA | 1530 | G |
| 22 | QV | 5 | G |
| 22 | QV | 7 | G |
| 22 | QV | 8 | U |
| 22 | QV | 18 | U |
| 22 | QV | 19 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | QV | 20 | G |
| 22 | QV | 21 | U |
| 22 | QV | 35 | C |
| 22 | QV | 36 | A |
| 22 | QV | 48 | U |
| 22 | QV | 49 | C |
| 22 | QV | 50 | G |
| 22 | QV | 53 | G |
| 22 | QV | 54 | G |
| 22 | QV | 55 | U |
| 22 | QV | 60 | A |
| 22 | QV | 76 | C |
| 22 | QW | 8 | U |
| 22 | QW | 9 | G |
| 22 | QW | 13 | C |
| 22 | QW | 14 | A |
| 22 | QW | 18 | U |
| 22 | QW | 19 | G |
| 22 | QW | 20 | G |
| 22 | QW | 21 | U |
| 22 | QW | 27 | G |
| 22 | QW | 32 | G |
| 22 | QW | 33 | C |
| 22 | QW | 34 | U |
| 22 | QW | 35 | C |
| 22 | QW | 36 | A |
| 22 | QW | 38 | A |
| 22 | QW | 39 | A |
| 22 | QW | 43 | G |
| 22 | QW | 46 | G |
| 22 | QW | 47 | G |
| 22 | QW | 48 | U |
| 22 | QW | 49 | C |
| 22 | QW | 50 | G |
| 22 | QW | 56 | U |
| 22 | QW | 57 | C |
| 22 | QW | 58 | A |
| 22 | QW | 59 | A |
| 22 | QW | 60 | A |
| 22 | QW | 61 | U |
| 22 | QW | 62 | C |
| 22 | QW | 74 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | QW | 75 | C |
| 24 | QY | 29 | G |
| 24 | QY | 30 | G |
| 25 | RA | 34 | C |
| 25 | RA | 35 | G |
| 25 | RA | 46 | C |
| 25 | RA | 51 | G |
| 25 | RA | 55 | G |
| 25 | RA | 61 | G |
| 25 | RA | 63 | U |
| 25 | RA | 72 | U |
| 25 | RA | 74 | A |
| 25 | RA | 75 | G |
| 25 | RA | 82 | G |
| 25 | RA | 101 | G |
| 25 | RA | 102 | G |
| 25 | RA | 103 | A |
| 25 | RA | 118 | A |
| 25 | RA | 120 | U |
| 25 | RA | 131 | G |
| 25 | RA | 138 | G |
| 25 | RA | 177 | G |
| 25 | RA | 181 | A |
| 25 | RA | 196 | A |
| 25 | RA | 199 | A |
| 25 | RA | 204 | A |
| 25 | RA | 205 | G |
| 25 | RA | 215 | G |
| 25 | RA | 216 | A |
| 25 | RA | 221 | A |
| 25 | RA | 222 | A |
| 25 | RA | 223 | A |
| 25 | RA | 228 | A |
| 25 | RA | 229 | A |
| 25 | RA | 230 | U |
| 25 | RA | 232 | G |
| 25 | RA | 242 | G |
| 25 | RA | 243 | U |
| 25 | RA | 248 | G |
| 25 | RA | 252 | G |
| 25 | RA | 265 | A |
| 25 | RA | 266 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 270(L) | U |
| 25 | RA | 270(M) | U |
| 25 | RA | 270(N) | G |
| 25 | RA | 270(P) | C |
| 25 | RA | 270(Y) | G |
| 25 | RA | 271(A) | C |
| 25 | RA | 271(C) | U |
| 25 | RA | 275 | G |
| 25 | RA | 276 | A |
| 25 | RA | 277 | C |
| 25 | RA | 299 | A |
| 25 | RA | 311 | A |
| 25 | RA | 323 | G |
| 25 | RA | 324 | A |
| 25 | RA | 329 | G |
| 25 | RA | 330 | A |
| 25 | RA | 342 | G |
| 25 | RA | 346 | A |
| 25 | RA | 352 | G |
| 25 | RA | 364 | C |
| 25 | RA | 371 | A |
| 25 | RA | 372 | G |
| 25 | RA | 373 | U |
| 25 | RA | 386 | G |
| 25 | RA | 405 | U |
| 25 | RA | 407 | G |
| 25 | RA | 411 | G |
| 25 | RA | 412 | A |
| 25 | RA | 428 | A |
| 25 | RA | 435 | C |
| 25 | RA | 444 | C |
| 25 | RA | 448 | U |
| 25 | RA | 455 | C |
| 25 | RA | 456 | C |
| 25 | RA | 457 | A |
| 25 | RA | 458 | G |
| 25 | RA | 470 | A |
| 25 | RA | 481 | G |
| 25 | RA | 491 | G |
| 25 | RA | 504 | U |
| 25 | RA | 505 | A |
| 25 | RA | 508 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 509 | C |
| 25 | RA | 513 | A |
| 25 | RA | 527 | C |
| 25 | RA | 529 | A |
| 25 | RA | 532 | A |
| 25 | RA | 533 | G |
| 25 | RA | 537 | C |
| 25 | RA | 539 | G |
| 25 | RA | 540 | G |
| 25 | RA | 546 | C |
| 25 | RA | 547 | A |
| 25 | RA | 554 | U |
| 25 | RA | 556 | G |
| 25 | RA | 563 | G |
| 25 | RA | 571 | A |
| 25 | RA | 573 | G |
| 25 | RA | 575 | A |
| 25 | RA | 588 | U |
| 25 | RA | 603 | A |
| 25 | RA | 607 | U |
| 25 | RA | 614 | U |
| 25 | RA | 615 | G |
| 25 | RA | 617 | G |
| 25 | RA | 621 | A |
| 25 | RA | 622 | G |
| 25 | RA | 627 | A |
| 25 | RA | 631 | A |
| 25 | RA | 637 | A |
| 25 | RA | 638 | G |
| 25 | RA | 645 | C |
| 25 | RA | 646 | A |
| 25 | RA | 647 | G |
| 25 | RA | 651 | G |
| 25 | RA | 652 | C |
| 25 | RA | 654 | A |
| 25 | RA | 654(A) | G |
| 25 | RA | 654(B) | C |
| 25 | RA | 658 | C |
| 25 | RA | 669 | G |
| 25 | RA | 686 | G |
| 25 | RA | 702 | G |
| 25 | RA | 708 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | RA | 722 | A |
| 25 | RA | 730 | C |
| 25 | RA | 748 | G |
| 25 | RA | 753 | C |
| 25 | RA | 776 | G |
| 25 | RA | 782 | A |
| 25 | RA | 784 | A |
| 25 | RA | 785 | G |
| 25 | RA | 790 | C |
| 25 | RA | 805 | G |
| 25 | RA | 812 | C |
| 25 | RA | 819 | A |
| 25 | RA | 827 | U |
| 25 | RA | 828 | U |
| 25 | RA | 830 | G |
| 25 | RA | 847 | U |
| 25 | RA | 856 | C |
| 25 | RA | 857 | C |
| 25 | RA | 859 | G |
| 25 | RA | 860 | U |
| 25 | RA | 869 | G |
| 25 | RA | 872 | A |
| 25 | RA | 880 | G |
| 25 | RA | 882 | G |
| 25 | RA | 884 | C |
| 25 | RA | 885 | C |
| 25 | RA | 886 | C |
| 25 | RA | 888 | C |
| 25 | RA | 889 | C |
| 25 | RA | 893 | C |
| 25 | RA | 896 | A |
| 25 | RA | 897 | C |
| 25 | RA | 900 | A |
| 25 | RA | 901 | A |
| 25 | RA | 904 | C |
| 25 | RA | 907 | U |
| 25 | RA | 910 | A |
| 25 | RA | 917 | A |
| 25 | RA | 930 | U |
| 25 | RA | 932 | G |
| 25 | RA | 938 | G |
| 25 | RA | 941 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | RA | 945 | A |
| 25 | RA | 946 | G |
| 25 | RA | 953 | A |
| 25 | RA | 957 | A |
| 25 | RA | 959 | A |
| 25 | RA | 961 | C |
| 25 | RA | 973 | A |
| 25 | RA | 974 | G |
| 25 | RA | 974(A) | C |
| 25 | RA | 975 | G |
| 25 | RA | 980 | A |
| 25 | RA | 983 | A |
| 25 | RA | 996 | A |
| 25 | RA | 1003 | G |
| 25 | RA | 1012 | U |
| 25 | RA | 1013 | C |
| 25 | RA | 1017 | G |
| 25 | RA | 1023 | U |
| 25 | RA | 1025 | G |
| 25 | RA | 1026 | U |
| 25 | RA | 1027 | A |
| 25 | RA | 1032 | A |
| 25 | RA | 1033 | U |
| 25 | RA | 1044 | G |
| 25 | RA | 1045 | A |
| 25 | RA | 1046 | A |
| 25 | RA | 1050 | A |
| 25 | RA | 1053 | C |
| 25 | RA | 1054 | A |
| 25 | RA | 1055 | G |
| 25 | RA | 1059 | G |
| 25 | RA | 1060 | U |
| 25 | RA | 1061 | U |
| 25 | RA | 1066 | U |
| 25 | RA | 1067 | A |
| 25 | RA | 1068 | G |
| 25 | RA | 1070 | A |
| 25 | RA | 1071 | G |
| 25 | RA | 1076 | C |
| 25 | RA | 1077 | A |
| 25 | RA | 1078 | U |
| 25 | RA | 1079 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1081 | U |
| 25 | RA | 1082 | U |
| 25 | RA | 1083 | U |
| 25 | RA | 1084 | A |
| 25 | RA | 1085 | A |
| 25 | RA | 1086 | A |
| 25 | RA | 1087 | G |
| 25 | RA | 1088 | A |
| 25 | RA | 1090 | U |
| 25 | RA | 1091 | G |
| 25 | RA | 1093 | G |
| 25 | RA | 1095 | A |
| 25 | RA | 1096 | A |
| 25 | RA | 1097 | U |
| 25 | RA | 1104 | C |
| 25 | RA | 1105 | U |
| 25 | RA | 1110 | G |
| 25 | RA | 1111 | A |
| 25 | RA | 1112 | G |
| 25 | RA | 1122 | G |
| 25 | RA | 1124 | C |
| 25 | RA | 1129 | A |
| 25 | RA | 1130 | U |
| 25 | RA | 1135 | C |
| 25 | RA | 1136 | G |
| 25 | RA | 1139 | G |
| 25 | RA | 1140 | C |
| 25 | RA | 1141 | U |
| 25 | RA | 1142(A) | A |
| 25 | RA | 1151 | G |
| 25 | RA | 1169 | G |
| 25 | RA | 1173 | G |
| 25 | RA | 1174 | A |
| 25 | RA | 1175 | U |
| 25 | RA | 1176 | G |
| 25 | RA | 1178 | C |
| 25 | RA | 1179 | C |
| 25 | RA | 1183 | G |
| 25 | RA | 1195 | G |
| 25 | RA | 1204 | A |
| 25 | RA | 1205 | U |
| 25 | RA | 1206 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1210 | A |
| 25 | RA | 1211 | U |
| 25 | RA | 1212 | G |
| 25 | RA | 1220 | A |
| 25 | RA | 1238 | G |
| 25 | RA | 1247 | A |
| 25 | RA | 1248 | G |
| 25 | RA | 1253 | A |
| 25 | RA | 1256 | G |
| 25 | RA | 1265 | A |
| 25 | RA | 1271 | G |
| 25 | RA | 1272 | A |
| 25 | RA | 1273 | U |
| 25 | RA | 1286 | A |
| 25 | RA | 1288 | U |
| 25 | RA | 1300 | U |
| 25 | RA | 1301 | A |
| 25 | RA | 1312 | U |
| 25 | RA | 1313 | U |
| 25 | RA | 1314 | C |
| 25 | RA | 1321 | A |
| 25 | RA | 1329 | U |
| 25 | RA | 1330 | C |
| 25 | RA | 1341 | U |
| 25 | RA | 1349 | A |
| 25 | RA | 1352 | U |
| 25 | RA | 1365 | A |
| 25 | RA | 1368 | G |
| 25 | RA | 1378 | A |
| 25 | RA | 1379 | A |
| 25 | RA | 1380 | G |
| 25 | RA | 1384 | A |
| 25 | RA | 1385 | G |
| 25 | RA | 1392 | A |
| 25 | RA | 1395 | A |
| 25 | RA | 1407 | C |
| 25 | RA | 1408 | C |
| 25 | RA | 1411 | C |
| 25 | RA | 1416 | G |
| 25 | RA | 1419 | A |
| 25 | RA | 1420 | U |
| 25 | RA | 1421 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1428 | C |
| 25 | RA | 1434 | A |
| 25 | RA | 1444(A) | A |
| 25 | RA | 1445 | C |
| 25 | RA | 1449 | A |
| 25 | RA | 1449(A) | G |
| 25 | RA | 1455 | G |
| 25 | RA | 1458 | C |
| 25 | RA | 1461 | G |
| 25 | RA | 1467 | C |
| 25 | RA | 1471 | A |
| 25 | RA | 1482 | U |
| 25 | RA | 1483 | G |
| 25 | RA | 1490 | A |
| 25 | RA | 1493 | C |
| 25 | RA | 1494 | A |
| 25 | RA | 1497 | U |
| 25 | RA | 1503 | U |
| 25 | RA | 1506 | C |
| 25 | RA | 1507 | A |
| 25 | RA | 1508 | A |
| 25 | RA | 1510 | A |
| 25 | RA | 1511 | A |
| 25 | RA | 1513 | C |
| 25 | RA | 1514 | U |
| 25 | RA | 1517 | G |
| 25 | RA | 1519 | G |
| 25 | RA | 1522 | G |
| 25 | RA | 1528 | A |
| 25 | RA | 1534 | G |
| 25 | RA | 1535 | U |
| 25 | RA | 1536 | A |
| 25 | RA | 1537 | C |
| 25 | RA | 1538 | G |
| 25 | RA | 1543 | A |
| 25 | RA | 1545 | A |
| 25 | RA | 1558 | A |
| 25 | RA | 1559 | G |
| 25 | RA | 1560 | G |
| 25 | RA | 1566 | A |
| 25 | RA | 1569 | A |
| 25 | RA | 1578 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1579 | A |
| 25 | RA | 1581 | G |
| 25 | RA | 1585 | C |
| 25 | RA | 1586 | A |
| 25 | RA | 1599 | C |
| 25 | RA | 1608 | A |
| 25 | RA | 1610 | A |
| 25 | RA | 1616 | A |
| 25 | RA | 1617 | C |
| 25 | RA | 1618 | A |
| 25 | RA | 1640 | C |
| 25 | RA | 1648 | C |
| 25 | RA | 1651 | G |
| 25 | RA | 1654 | A |
| 25 | RA | 1665 | A |
| 25 | RA | 1667 | G |
| 25 | RA | 1668 | A |
| 25 | RA | 1674 | G |
| 25 | RA | 1675 | C |
| 25 | RA | 1678 | G |
| 25 | RA | 1695 | G |
| 25 | RA | 1725 | G |
| 25 | RA | 1728 | G |
| 25 | RA | 1729 | A |
| 25 | RA | 1730 | U |
| 25 | RA | 1731 | G |
| 25 | RA | 1732 | A |
| 25 | RA | 1733 | G |
| 25 | RA | 1742 | C |
| 25 | RA | 1743 | G |
| 25 | RA | 1756 | G |
| 25 | RA | 1762 | A |
| 25 | RA | 1763 | G |
| 25 | RA | 1764 | G |
| 25 | RA | 1773 | A |
| 25 | RA | 1779 | U |
| 25 | RA | 1780 | A |
| 25 | RA | 1781 | C |
| 25 | RA | 1782 | C |
| 25 | RA | 1787 | A |
| 25 | RA | 1791 | A |
| 25 | RA | 1799 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 1800 | C |
| 25 | RA | 1801 | G |
| 25 | RA | 1816 | G |
| 25 | RA | 1820 | U |
| 25 | RA | 1829 | A |
| 25 | RA | 1835 | G |
| 25 | RA | 1847 | A |
| 25 | RA | 1848 | A |
| 25 | RA | 1858 | G |
| 25 | RA | 1869 | G |
| 25 | RA | 1870 | C |
| 25 | RA | 1872 | A |
| 25 | RA | 1878 | G |
| 25 | RA | 1882 | C |
| 25 | RA | 1888 | G |
| 25 | RA | 1889 | A |
| 25 | RA | 1906 | G |
| 25 | RA | 1927 | A |
| 25 | RA | 1929 | G |
| 25 | RA | 1930 | G |
| 25 | RA | 1931 | U |
| 25 | RA | 1936 | A |
| 25 | RA | 1937 | A |
| 25 | RA | 1938 | A |
| 25 | RA | 1939 | U |
| 25 | RA | 1955 | U |
| 25 | RA | 1963 | U |
| 25 | RA | 1964 | G |
| 25 | RA | 1967 | C |
| 25 | RA | 1969 | A |
| 25 | RA | 1970 | A |
| 25 | RA | 1971 | A |
| 25 | RA | 1972 | A |
| 25 | RA | 1982 | C |
| 25 | RA | 1992 | G |
| 25 | RA | 1993 | U |
| 25 | RA | 1996 | C |
| 25 | RA | 2013 | A |
| 25 | RA | 2020 | A |
| 25 | RA | 2021 | C |
| 25 | RA | 2023 | G |
| 25 | RA | 2031 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 2032 | G |
| 25 | RA | 2033 | A |
| 25 | RA | 2043 | C |
| 25 | RA | 2052 | G |
| 25 | RA | 2055 | C |
| 25 | RA | 2056 | G |
| 25 | RA | 2059 | A |
| 25 | RA | 2060 | A |
| 25 | RA | 2061 | G |
| 25 | RA | 2062 | A |
| 25 | RA | 2069 | G |
| 25 | RA | 2093 | G |
| 25 | RA | 2111 | C |
| 25 | RA | 2113 | U |
| 25 | RA | 2114 | A |
| 25 | RA | 2115 | G |
| 25 | RA | 2116 | G |
| 25 | RA | 2117 | A |
| 25 | RA | 2119 | A |
| 25 | RA | 2123 | G |
| 25 | RA | 2126 | A |
| 25 | RA | 2127 | G |
| 25 | RA | 2128 | C |
| 25 | RA | 2131 | G |
| 25 | RA | 2132 | U |
| 25 | RA | 2135 | A |
| 25 | RA | 2136 | C |
| 25 | RA | 2146 | C |
| 25 | RA | 2147 | G |
| 25 | RA | 2148 | G |
| 25 | RA | 2157 | G |
| 25 | RA | 2158 | A |
| 25 | RA | 2161 | C |
| 25 | RA | 2166 | G |
| 25 | RA | 2168 | G |
| 25 | RA | 2169 | A |
| 25 | RA | 2173 | A |
| 25 | RA | 2176 | A |
| 25 | RA | 2189 | U |
| 25 | RA | 2190 | G |
| 25 | RA | 2198 | A |
| 25 | RA | 2199 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2210 | G |
| 25 | RA | 2211 | G |
| 25 | RA | 2212 | A |
| 25 | RA | 2213 | U |
| 25 | RA | 2215 | G |
| 25 | RA | 2225 | A |
| 25 | RA | 2238 | G |
| 25 | RA | 2239 | G |
| 25 | RA | 2243 | U |
| 25 | RA | 2266 | A |
| 25 | RA | 2275 | C |
| 25 | RA | 2280 | G |
| 25 | RA | 2283 | C |
| 25 | RA | 2287 | A |
| 25 | RA | 2288 | A |
| 25 | RA | 2307 | G |
| 25 | RA | 2308 | G |
| 25 | RA | 2312 | U |
| 25 | RA | 2319 | G |
| 25 | RA | 2320 | A |
| 25 | RA | 2325 | G |
| 25 | RA | 2335 | A |
| 25 | RA | 2342 | C |
| 25 | RA | 2345 | G |
| 25 | RA | 2346 | A |
| 25 | RA | 2347 | C |
| 25 | RA | 2350 | C |
| 25 | RA | 2354 | G |
| 25 | RA | 2358 | G |
| 25 | RA | 2383 | G |
| 25 | RA | 2385 | C |
| 25 | RA | 2392 | A |
| 25 | RA | 2394 | C |
| 25 | RA | 2402 | C |
| 25 | RA | 2403 | C |
| 25 | RA | 2406 | U |
| 25 | RA | 2423 | U |
| 25 | RA | 2424 | C |
| 25 | RA | 2425 | A |
| 25 | RA | 2429 | G |
| 25 | RA | 2430 | A |
| 25 | RA | 2434 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2435 | A |
| 25 | RA | 2439 | A |
| 25 | RA | 2440 | C |
| 25 | RA | 2441 | C |
| 25 | RA | 2447 | G |
| 25 | RA | 2448 | A |
| 25 | RA | 2465 | C |
| 25 | RA | 2466 | C |
| 25 | RA | 2467 | C |
| 25 | RA | 2468 | G |
| 25 | RA | 2469 | A |
| 25 | RA | 2470 | G |
| 25 | RA | 2474 | C |
| 25 | RA | 2475 | C |
| 25 | RA | 2476 | A |
| 25 | RA | 2478 | A |
| 25 | RA | 2479 | G |
| 25 | RA | 2482 | G |
| 25 | RA | 2494 | G |
| 25 | RA | 2502 | G |
| 25 | RA | 2505 | G |
| 25 | RA | 2518 | A |
| 25 | RA | 2519 | U |
| 25 | RA | 2527 | C |
| 25 | RA | 2529 | G |
| 25 | RA | 2542 | A |
| 25 | RA | 2543 | G |
| 25 | RA | 2554 | U |
| 25 | RA | 2564 | A |
| 25 | RA | 2567 | G |
| 25 | RA | 2572 | A |
| 25 | RA | 2585 | U |
| 25 | RA | 2602 | A |
| 25 | RA | 2609 | U |
| 25 | RA | 2611 | U |
| 25 | RA | 2612 | C |
| 25 | RA | 2614 | A |
| 25 | RA | 2615 | U |
| 25 | RA | 2621 | A |
| 25 | RA | 2623 | G |
| 25 | RA | 2629 | A |
| 25 | RA | 2641 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | RA | 2642 | G |
| 25 | RA | 2655 | G |
| 25 | RA | 2665 | A |
| 25 | RA | 2673 | G |
| 25 | RA | 2682 | U |
| 25 | RA | 2689 | U |
| 25 | RA | 2690 | C |
| 25 | RA | 2702 | U |
| 25 | RA | 2707 | G |
| 25 | RA | 2712 | U |
| 25 | RA | 2712(A) | A |
| 25 | RA | 2713 | A |
| 25 | RA | 2714 | G |
| 25 | RA | 2726 | U |
| 25 | RA | 2732 | G |
| 25 | RA | 2733 | A |
| 25 | RA | 2739 | U |
| 25 | RA | 2743 | C |
| 25 | RA | 2744 | G |
| 25 | RA | 2748 | A |
| 25 | RA | 2752 | C |
| 25 | RA | 2753 | A |
| 25 | RA | 2754 | U |
| 25 | RA | 2756 | U |
| 25 | RA | 2757 | A |
| 25 | RA | 2758 | A |
| 25 | RA | 2761 | G |
| 25 | RA | 2764 | A |
| 25 | RA | 2765 | A |
| 25 | RA | 2766 | G |
| 25 | RA | 2771 | C |
| 25 | RA | 2777 | G |
| 25 | RA | 2778 | A |
| 25 | RA | 2779 | U |
| 25 | RA | 2780 | G |
| 25 | RA | 2789 | C |
| 25 | RA | 2790 | A |
| 25 | RA | 2791 | C |
| 25 | RA | 2797 | U |
| 25 | RA | 2807 | G |
| 25 | RA | 2818 | G |
| 25 | RA | 2820 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | RA | 2821 | A |
| 25 | RA | 2832 | U |
| 25 | RA | 2833 | G |
| 25 | RA | 2834 | G |
| 25 | RA | 2835 | A |
| 25 | RA | 2847 | U |
| 25 | RA | 2849 | U |
| 25 | RA | 2872 | G |
| 25 | RA | 2873 | A |
| 25 | RA | 2880 | C |
| 25 | RA | 2886 | G |
| 25 | RA | 2891 | G |
| 25 | RA | 2892 | A |
| 25 | RA | 2894 | G |
| 26 | RB | 9 | G |
| 26 | RB | 13 | A |
| 26 | RB | 15 | A |
| 26 | RB | 16 | G |
| 26 | RB | 22 | U |
| 26 | RB | 25 | A |
| 26 | RB | 32 | C |
| 26 | RB | 41 | U |
| 26 | RB | 42 | C |
| 26 | RB | 45 | A |
| 26 | RB | 56 | G |
| 26 | RB | 66 | A |
| 26 | RB | 67 | G |
| 26 | RB | 73 | A |
| 26 | RB | 81 | G |
| 26 | RB | 82 | G |
| 26 | RB | 109 | G |
| 1 | XA | 6 | G |
| 1 | XA | 9 | G |
| 1 | XA | 32 | A |
| 1 | XA | 39 | G |
| 1 | XA | 47 | C |
| 1 | XA | 48 | C |
| 1 | XA | 50 | A |
| 1 | XA | 51 | A |
| 1 | XA | 61 | G |
| 1 | XA | 65 | U |
| 1 | XA | 66 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | XA | 76 | G |
| 1 | XA | 79 | G |
| 1 | XA | 81 | G |
| 1 | XA | 89 | U |
| 1 | XA | 90 | C |
| 1 | XA | 91 | C |
| 1 | XA | 92 | G |
| 1 | XA | 95 | G |
| 1 | XA | 101 | A |
| 1 | XA | 108 | G |
| 1 | XA | 116 | A |
| 1 | XA | 121 | C |
| 1 | XA | 122 | G |
| 1 | XA | 129(A) | G |
| 1 | XA | 130 | A |
| 1 | XA | 144 | G |
| 1 | XA | 147 | G |
| 1 | XA | 151 | A |
| 1 | XA | 163 | C |
| 1 | XA | 169 | C |
| 1 | XA | 172 | A |
| 1 | XA | 174 | C |
| 1 | XA | 190 | G |
| 1 | XA | 191(A) | G |
| 1 | XA | 195 | A |
| 1 | XA | 197 | A |
| 1 | XA | 209 | U |
| 1 | XA | 222 | U |
| 1 | XA | 244 | U |
| 1 | XA | 245 | C |
| 1 | XA | 247 | G |
| 1 | XA | 251 | G |
| 1 | XA | 262 | A |
| 1 | XA | 267 | C |
| 1 | XA | 270 | A |
| 1 | XA | 281 | G |
| 1 | XA | 289 | G |
| 1 | XA | 314 | C |
| 1 | XA | 317 | G |
| 1 | XA | 321 | A |
| 1 | XA | 328 | C |
| 1 | XA | 329 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 332 | G |
| 1 | XA | 345 | C |
| 1 | XA | 346 | G |
| 1 | XA | 347 | G |
| 1 | XA | 351 | G |
| 1 | XA | 352 | C |
| 1 | XA | 353 | A |
| 1 | XA | 354 | G |
| 1 | XA | 356 | A |
| 1 | XA | 367 | U |
| 1 | XA | 372 | C |
| 1 | XA | 373 | A |
| 1 | XA | 384 | G |
| 1 | XA | 388 | G |
| 1 | XA | 389 | A |
| 1 | XA | 390 | C |
| 1 | XA | 397 | A |
| 1 | XA | 398 | C |
| 1 | XA | 406 | G |
| 1 | XA | 411 | A |
| 1 | XA | 412 | A |
| 1 | XA | 413 | G |
| 1 | XA | 421 | U |
| 1 | XA | 422 | C |
| 1 | XA | 423 | G |
| 1 | XA | 424 | G |
| 1 | XA | 429 | U |
| 1 | XA | 430 | A |
| 1 | XA | 440 | A |
| 1 | XA | 442 | C |
| 1 | XA | 452 | A |
| 1 | XA | 466 | C |
| 1 | XA | 467 | G |
| 1 | XA | 482 | A |
| 1 | XA | 485 | G |
| 1 | XA | 486 | U |
| 1 | XA | 496 | A |
| 1 | XA | 497 | U |
| 1 | XA | 509 | A |
| 1 | XA | 510 | A |
| 1 | XA | 511 | C |
| 1 | XA | 518 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | XA | 521 | G |
| 1 | XA | 524 | G |
| 1 | XA | 527 | G |
| 1 | XA | 531 | U |
| 1 | XA | 532 | A |
| 1 | XA | 533 | A |
| 1 | XA | 545 | C |
| 1 | XA | 547 | A |
| 1 | XA | 548 | G |
| 1 | XA | 559 | A |
| 1 | XA | 561 | U |
| 1 | XA | 564 | C |
| 1 | XA | 568 | G |
| 1 | XA | 572 | A |
| 1 | XA | 573 | A |
| 1 | XA | 576 | G |
| 1 | XA | 577 | G |
| 1 | XA | 579 | G |
| 1 | XA | 618 | C |
| 1 | XA | 630 | G |
| 1 | XA | 631 | G |
| 1 | XA | 632 | A |
| 1 | XA | 633 | G |
| 1 | XA | 653 | A |
| 1 | XA | 665 | A |
| 1 | XA | 671 | G |
| 1 | XA | 688 | G |
| 1 | XA | 702 | A |
| 1 | XA | 704 | A |
| 1 | XA | 721 | G |
| 1 | XA | 723 | U |
| 1 | XA | 731 | G |
| 1 | XA | 749 | C |
| 1 | XA | 754 | C |
| 1 | XA | 755 | G |
| 1 | XA | 774 | G |
| 1 | XA | 777 | A |
| 1 | XA | 792 | A |
| 1 | XA | 793 | U |
| 1 | XA | 794 | A |
| 1 | XA | 813 | U |
| 1 | XA | 817 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 818 | G |
| 1 | XA | 821 | G |
| 1 | XA | 828 | A |
| 1 | XA | 841 | U |
| 1 | XA | 843 | U |
| 1 | XA | 848 | C |
| 1 | XA | 859 | A |
| 1 | XA | 871 | U |
| 1 | XA | 872 | A |
| 1 | XA | 902 | G |
| 1 | XA | 914 | A |
| 1 | XA | 926 | G |
| 1 | XA | 927 | G |
| 1 | XA | 934 | C |
| 1 | XA | 935 | A |
| 1 | XA | 940 | C |
| 1 | XA | 942 | G |
| 1 | XA | 958 | A |
| 1 | XA | 960 | U |
| 1 | XA | 968 | A |
| 1 | XA | 969 | A |
| 1 | XA | 971 | G |
| 1 | XA | 972 | C |
| 1 | XA | 974 | A |
| 1 | XA | 975 | A |
| 1 | XA | 976 | G |
| 1 | XA | 977 | A |
| 1 | XA | 980 | C |
| 1 | XA | 991 | U |
| 1 | XA | 992 | U |
| 1 | XA | 993 | G |
| 1 | XA | 1004 | A |
| 1 | XA | 1006 | C |
| 1 | XA | 1009 | G |
| 1 | XA | 1024 | G |
| 1 | XA | 1025 | U |
| 1 | XA | 1028 | C |
| 1 | XA | 1029 | G |
| 1 | XA | 1032(A) | G |
| 1 | XA | 1039 | C |
| 1 | XA | 1040 | U |
| 1 | XA | 1053 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | XA | 1054 | C |
| 1 | XA | 1055 | A |
| 1 | XA | 1064 | G |
| 1 | XA | 1065 | U |
| 1 | XA | 1066 | C |
| 1 | XA | 1081 | G |
| 1 | XA | 1085 | U |
| 1 | XA | 1094 | G |
| 1 | XA | 1095 | U |
| 1 | XA | 1101 | A |
| 1 | XA | 1124 | G |
| 1 | XA | 1125 | U |
| 1 | XA | 1126 | U |
| 1 | XA | 1127 | G |
| 1 | XA | 1130 | A |
| 1 | XA | 1131 | G |
| 1 | XA | 1136 | U |
| 1 | XA | 1137 | C |
| 1 | XA | 1138 | G |
| 1 | XA | 1139 | G |
| 1 | XA | 1146 | A |
| 1 | XA | 1152 | A |
| 1 | XA | 1157 | A |
| 1 | XA | 1158 | C |
| 1 | XA | 1159 | U |
| 1 | XA | 1160 | G |
| 1 | XA | 1176 | A |
| 1 | XA | 1177 | G |
| 1 | XA | 1181 | G |
| 1 | XA | 1183 | A |
| 1 | XA | 1184 | G |
| 1 | XA | 1187 | G |
| 1 | XA | 1196 | U |
| 1 | XA | 1201 | A |
| 1 | XA | 1212 | U |
| 1 | XA | 1213 | A |
| 1 | XA | 1225 | A |
| 1 | XA | 1238 | A |
| 1 | XA | 1240 | U |
| 1 | XA | 1241 | G |
| 1 | XA | 1256 | A |
| 1 | XA | 1257 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | XA | 1258 | G |
| 1 | XA | 1263 | C |
| 1 | XA | 1270 | C |
| 1 | XA | 1273 | G |
| 1 | XA | 1280 | A |
| 1 | XA | 1281 | U |
| 1 | XA | 1282 | C |
| 1 | XA | 1286 | A |
| 1 | XA | 1287 | A |
| 1 | XA | 1298 | C |
| 1 | XA | 1300 | G |
| 1 | XA | 1301 | U |
| 1 | XA | 1302 | U |
| 1 | XA | 1303 | C |
| 1 | XA | 1305 | G |
| 1 | XA | 1318 | A |
| 1 | XA | 1319 | A |
| 1 | XA | 1320 | C |
| 1 | XA | 1321 | C |
| 1 | XA | 1322 | C |
| 1 | XA | 1323 | G |
| 1 | XA | 1331 | G |
| 1 | XA | 1336 | C |
| 1 | XA | 1337 | G |
| 1 | XA | 1347 | G |
| 1 | XA | 1353 | G |
| 1 | XA | 1362(A) | C |
| 1 | XA | 1363 | A |
| 1 | XA | 1364 | U |
| 1 | XA | 1378 | C |
| 1 | XA | 1397 | C |
| 1 | XA | 1398 | A |
| 1 | XA | 1419 | G |
| 1 | XA | 1442 | G |
| 1 | XA | 1446 | A |
| 1 | XA | 1447 | G |
| 1 | XA | 1452 | C |
| 1 | XA | 1453 | G |
| 1 | XA | 1454 | G |
| 1 | XA | 1492 | A |
| 1 | XA | 1497 | G |
| 1 | XA | 1499 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | XA | 1502 | A |
| 1 | XA | 1503 | A |
| 1 | XA | 1504 | G |
| 1 | XA | 1506 | U |
| 1 | XA | 1507 | A |
| 1 | XA | 1517 | G |
| 1 | XA | 1520 | G |
| 1 | XA | 1529 | G |
| 1 | XA | 1530 | G |
| 22 | XV | 5 | G |
| 22 | XV | 7 | G |
| 22 | XV | 8 | U |
| 22 | XV | 18 | U |
| 22 | XV | 20 | G |
| 22 | XV | 21 | U |
| 22 | XV | 23 | G |
| 22 | XV | 35 | C |
| 22 | XV | 36 | A |
| 22 | XV | 48 | U |
| 22 | XV | 49 | C |
| 22 | XV | 50 | G |
| 22 | XV | 51 | U |
| 22 | XV | 53 | G |
| 22 | XV | 54 | G |
| 22 | XV | 55 | U |
| 22 | XV | 66 | C |
| 22 | XV | 76 | C |
| 22 | XW | 8 | U |
| 22 | XW | 9 | G |
| 22 | XW | 10 | G |
| 22 | XW | 13 | C |
| 22 | XW | 14 | A |
| 22 | XW | 18 | U |
| 22 | XW | 19 | G |
| 22 | XW | 20 | G |
| 22 | XW | 21 | U |
| 22 | XW | 27 | G |
| 22 | XW | 32 | G |
| 22 | XW | 33 | C |
| 22 | XW | 34 | U |
| 22 | XW | 35 | C |
| 22 | XW | 36 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | XW | 38 | A |
| 22 | XW | 39 | A |
| 22 | XW | 43 | G |
| 22 | XW | 46 | G |
| 22 | XW | 47 | G |
| 22 | XW | 48 | U |
| 22 | XW | 49 | C |
| 22 | XW | 50 | G |
| 22 | XW | 56 | U |
| 22 | XW | 57 | C |
| 22 | XW | 58 | A |
| 22 | XW | 59 | A |
| 22 | XW | 60 | A |
| 22 | XW | 61 | U |
| 22 | XW | 62 | C |
| 22 | XW | 74 | A |
| 22 | XW | 75 | C |
| 23 | XX | 14 | A |
| 23 | XX | 15 | A |
| 23 | XX | 22 | A |
| 24 | XY | 29 | G |
| 24 | XY | 30 | G |
| 25 | YA | 13 | A |
| 25 | YA | 34 | C |
| 25 | YA | 35 | G |
| 25 | YA | 46 | C |
| 25 | YA | 55 | G |
| 25 | YA | 61 | G |
| 25 | YA | 63 | U |
| 25 | YA | 72 | U |
| 25 | YA | 74 | A |
| 25 | YA | 75 | G |
| 25 | YA | 96 | G |
| 25 | YA | 101 | G |
| 25 | YA | 102 | G |
| 25 | YA | 103 | A |
| 25 | YA | 118 | A |
| 25 | YA | 120 | U |
| 25 | YA | 125 | G |
| 25 | YA | 131 | G |
| 25 | YA | 161 | U |
| 25 | YA | 162 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 181 | A |
| 25 | YA | 188 | G |
| 25 | YA | 196 | A |
| 25 | YA | 199 | A |
| 25 | YA | 214 | G |
| 25 | YA | 216 | A |
| 25 | YA | 221 | A |
| 25 | YA | 222 | A |
| 25 | YA | 223 | A |
| 25 | YA | 228 | A |
| 25 | YA | 229 | A |
| 25 | YA | 230 | U |
| 25 | YA | 232 | G |
| 25 | YA | 233 | A |
| 25 | YA | 242 | G |
| 25 | YA | 243 | U |
| 25 | YA | 248 | G |
| 25 | YA | 252 | G |
| 25 | YA | 265 | A |
| 25 | YA | 266 | G |
| 25 | YA | 270(L) | U |
| 25 | YA | 270(M) | U |
| 25 | YA | 270(N) | G |
| 25 | YA | 270(P) | C |
| 25 | YA | 271(A) | C |
| 25 | YA | 271(B) | G |
| 25 | YA | 271(C) | U |
| 25 | YA | 271 | G |
| 25 | YA | 274 | G |
| 25 | YA | 275 | G |
| 25 | YA | 276 | A |
| 25 | YA | 278 | A |
| 25 | YA | 279 | C |
| 25 | YA | 283 | A |
| 25 | YA | 299 | A |
| 25 | YA | 300 | A |
| 25 | YA | 311 | A |
| 25 | YA | 312 | G |
| 25 | YA | 316 | C |
| 25 | YA | 323 | G |
| 25 | YA | 324 | A |
| 25 | YA | 329 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 330 | A |
| 25 | YA | 332 | A |
| 25 | YA | 342 | G |
| 25 | YA | 343 | C |
| 25 | YA | 352 | G |
| 25 | YA | 363 | G |
| 25 | YA | 363(E) | U |
| 25 | YA | 364 | C |
| 25 | YA | 371 | A |
| 25 | YA | 372 | G |
| 25 | YA | 373 | U |
| 25 | YA | 380 | U |
| 25 | YA | 386 | G |
| 25 | YA | 387 | U |
| 25 | YA | 405 | U |
| 25 | YA | 406 | G |
| 25 | YA | 407 | G |
| 25 | YA | 411 | G |
| 25 | YA | 412 | A |
| 25 | YA | 421 | U |
| 25 | YA | 428 | A |
| 25 | YA | 444 | C |
| 25 | YA | 448 | U |
| 25 | YA | 451 | C |
| 25 | YA | 456 | C |
| 25 | YA | 457 | A |
| 25 | YA | 458 | G |
| 25 | YA | 470 | A |
| 25 | YA | 481 | G |
| 25 | YA | 496 | G |
| 25 | YA | 501 | A |
| 25 | YA | 504 | U |
| 25 | YA | 505 | A |
| 25 | YA | 509 | C |
| 25 | YA | 512 | G |
| 25 | YA | 518 | G |
| 25 | YA | 531 | C |
| 25 | YA | 532 | A |
| 25 | YA | 533 | G |
| 25 | YA | 537 | C |
| 25 | YA | 539 | G |
| 25 | YA | 540 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 546 | C |
| 25 | YA | 547 | A |
| 25 | YA | 563 | G |
| 25 | YA | 573 | G |
| 25 | YA | 575 | A |
| 25 | YA | 588 | U |
| 25 | YA | 603 | A |
| 25 | YA | 607 | U |
| 25 | YA | 614 | U |
| 25 | YA | 615 | G |
| 25 | YA | 617 | G |
| 25 | YA | 622 | G |
| 25 | YA | 627 | A |
| 25 | YA | 634 | C |
| 25 | YA | 637 | A |
| 25 | YA | 638 | G |
| 25 | YA | 645 | C |
| 25 | YA | 646 | A |
| 25 | YA | 651 | G |
| 25 | YA | 654 | A |
| 25 | YA | 654(A) | G |
| 25 | YA | 668 | G |
| 25 | YA | 686 | G |
| 25 | YA | 717 | G |
| 25 | YA | 722 | A |
| 25 | YA | 730 | C |
| 25 | YA | 747 | U |
| 25 | YA | 753 | C |
| 25 | YA | 764 | A |
| 25 | YA | 765 | G |
| 25 | YA | 782 | A |
| 25 | YA | 784 | A |
| 25 | YA | 785 | G |
| 25 | YA | 790 | C |
| 25 | YA | 792 | G |
| 25 | YA | 805 | G |
| 25 | YA | 812 | C |
| 25 | YA | 819 | A |
| 25 | YA | 827 | U |
| 25 | YA | 828 | U |
| 25 | YA | 831 | G |
| 25 | YA | 847 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 856 | C |
| 25 | YA | 857 | C |
| 25 | YA | 860 | U |
| 25 | YA | 881 | G |
| 25 | YA | 884 | C |
| 25 | YA | 885 | C |
| 25 | YA | 886 | C |
| 25 | YA | 888 | C |
| 25 | YA | 889 | C |
| 25 | YA | 896 | A |
| 25 | YA | 899 | A |
| 25 | YA | 900 | A |
| 25 | YA | 906 | G |
| 25 | YA | 907 | U |
| 25 | YA | 910 | A |
| 25 | YA | 914 | C |
| 25 | YA | 915 | C |
| 25 | YA | 917 | A |
| 25 | YA | 930 | U |
| 25 | YA | 932 | G |
| 25 | YA | 941 | A |
| 25 | YA | 945 | A |
| 25 | YA | 946 | G |
| 25 | YA | 953 | A |
| 25 | YA | 959 | A |
| 25 | YA | 961 | C |
| 25 | YA | 965 | C |
| 25 | YA | 974 | G |
| 25 | YA | 974(A) | C |
| 25 | YA | 975 | G |
| 25 | YA | 980 | A |
| 25 | YA | 983 | A |
| 25 | YA | 996 | A |
| 25 | YA | 1003 | G |
| 25 | YA | 1009 | A |
| 25 | YA | 1011 | G |
| 25 | YA | 1012 | U |
| 25 | YA | 1013 | C |
| 25 | YA | 1015 | G |
| 25 | YA | 1017 | G |
| 25 | YA | 1023 | U |
| 25 | YA | 1025 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | YA | 1026 | U |
| 25 | YA | 1027 | A |
| 25 | YA | 1033 | U |
| 25 | YA | 1045 | A |
| 25 | YA | 1046 | A |
| 25 | YA | 1050 | A |
| 25 | YA | 1054 | A |
| 25 | YA | 1059 | G |
| 25 | YA | 1060 | U |
| 25 | YA | 1061 | U |
| 25 | YA | 1065 | U |
| 25 | YA | 1066 | U |
| 25 | YA | 1067 | A |
| 25 | YA | 1068 | G |
| 25 | YA | 1071 | G |
| 25 | YA | 1073 | A |
| 25 | YA | 1077 | A |
| 25 | YA | 1078 | U |
| 25 | YA | 1079 | C |
| 25 | YA | 1082 | U |
| 25 | YA | 1083 | U |
| 25 | YA | 1084 | A |
| 25 | YA | 1085 | A |
| 25 | YA | 1086 | A |
| 25 | YA | 1088 | A |
| 25 | YA | 1093 | G |
| 25 | YA | 1095 | A |
| 25 | YA | 1096 | A |
| 25 | YA | 1097 | U |
| 25 | YA | 1103 | A |
| 25 | YA | 1104 | C |
| 25 | YA | 1110 | G |
| 25 | YA | 1111 | A |
| 25 | YA | 1129 | A |
| 25 | YA | 1130 | U |
| 25 | YA | 1135 | C |
| 25 | YA | 1136 | G |
| 25 | YA | 1139 | G |
| 25 | YA | 1142 | U |
| 25 | YA | 1142(A) | A |
| 25 | YA | 1151 | G |
| 25 | YA | 1168 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1170 | G |
| 25 | YA | 1173 | G |
| 25 | YA | 1174 | A |
| 25 | YA | 1175 | U |
| 25 | YA | 1176 | G |
| 25 | YA | 1179 | C |
| 25 | YA | 1195 | G |
| 25 | YA | 1204 | A |
| 25 | YA | 1205 | U |
| 25 | YA | 1206 | G |
| 25 | YA | 1210 | A |
| 25 | YA | 1211 | U |
| 25 | YA | 1220 | A |
| 25 | YA | 1236 | G |
| 25 | YA | 1238 | G |
| 25 | YA | 1250 | G |
| 25 | YA | 1252 | G |
| 25 | YA | 1253 | A |
| 25 | YA | 1256 | G |
| 25 | YA | 1265 | A |
| 25 | YA | 1272 | A |
| 25 | YA | 1273 | U |
| 25 | YA | 1300 | U |
| 25 | YA | 1301 | A |
| 25 | YA | 1319 | G |
| 25 | YA | 1329 | U |
| 25 | YA | 1349 | A |
| 25 | YA | 1352 | U |
| 25 | YA | 1365 | A |
| 25 | YA | 1368 | G |
| 25 | YA | 1378 | A |
| 25 | YA | 1379 | A |
| 25 | YA | 1380 | G |
| 25 | YA | 1384 | A |
| 25 | YA | 1385 | G |
| 25 | YA | 1388 | G |
| 25 | YA | 1391 | U |
| 25 | YA | 1395 | A |
| 25 | YA | 1407 | C |
| 25 | YA | 1411 | C |
| 25 | YA | 1416 | G |
| 25 | YA | 1419 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | YA | 1420 | U |
| 25 | YA | 1421 | G |
| 25 | YA | 1428 | C |
| 25 | YA | 1444(A) | A |
| 25 | YA | 1445 | C |
| 25 | YA | 1449 | A |
| 25 | YA | 1449(A) | G |
| 25 | YA | 1455 | G |
| 25 | YA | 1458 | C |
| 25 | YA | 1460 | A |
| 25 | YA | 1461 | G |
| 25 | YA | 1467 | C |
| 25 | YA | 1471 | A |
| 25 | YA | 1474 | C |
| 25 | YA | 1480 | G |
| 25 | YA | 1482 | U |
| 25 | YA | 1483 | G |
| 25 | YA | 1490 | A |
| 25 | YA | 1493 | C |
| 25 | YA | 1496 | A |
| 25 | YA | 1497 | U |
| 25 | YA | 1507 | A |
| 25 | YA | 1508 | A |
| 25 | YA | 1510 | A |
| 25 | YA | 1511 | A |
| 25 | YA | 1514 | U |
| 25 | YA | 1522 | G |
| 25 | YA | 1534 | G |
| 25 | YA | 1535 | U |
| 25 | YA | 1536 | A |
| 25 | YA | 1537 | C |
| 25 | YA | 1540 | G |
| 25 | YA | 1543 | A |
| 25 | YA | 1544 | C |
| 25 | YA | 1545 | A |
| 25 | YA | 1547 | C |
| 25 | YA | 1558 | A |
| 25 | YA | 1559 | G |
| 25 | YA | 1560 | G |
| 25 | YA | 1566 | A |
| 25 | YA | 1569 | A |
| 25 | YA | 1578 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1579 | A |
| 25 | YA | 1581 | G |
| 25 | YA | 1585 | C |
| 25 | YA | 1586 | A |
| 25 | YA | 1591 | G |
| 25 | YA | 1592 | C |
| 25 | YA | 1598 | C |
| 25 | YA | 1608 | A |
| 25 | YA | 1609 | A |
| 25 | YA | 1616 | A |
| 25 | YA | 1617 | C |
| 25 | YA | 1639 | U |
| 25 | YA | 1640 | C |
| 25 | YA | 1646 | C |
| 25 | YA | 1648 | C |
| 25 | YA | 1654 | A |
| 25 | YA | 1660 | C |
| 25 | YA | 1674 | G |
| 25 | YA | 1688 | U |
| 25 | YA | 1695 | G |
| 25 | YA | 1698 | A |
| 25 | YA | 1699 | G |
| 25 | YA | 1700 | A |
| 25 | YA | 1725 | G |
| 25 | YA | 1728 | G |
| 25 | YA | 1729 | A |
| 25 | YA | 1731 | G |
| 25 | YA | 1742 | C |
| 25 | YA | 1743 | G |
| 25 | YA | 1749 | A |
| 25 | YA | 1754 | C |
| 25 | YA | 1757 | U |
| 25 | YA | 1763 | G |
| 25 | YA | 1764 | G |
| 25 | YA | 1773 | A |
| 25 | YA | 1780 | A |
| 25 | YA | 1781 | C |
| 25 | YA | 1782 | C |
| 25 | YA | 1787 | A |
| 25 | YA | 1791 | A |
| 25 | YA | 1799 | G |
| 25 | YA | 1800 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 1801 | G |
| 25 | YA | 1816 | G |
| 25 | YA | 1820 | U |
| 25 | YA | 1829 | A |
| 25 | YA | 1835 | G |
| 25 | YA | 1847 | A |
| 25 | YA | 1848 | A |
| 25 | YA | 1858 | G |
| 25 | YA | 1864 | U |
| 25 | YA | 1869 | G |
| 25 | YA | 1870 | C |
| 25 | YA | 1872 | A |
| 25 | YA | 1878 | G |
| 25 | YA | 1882 | C |
| 25 | YA | 1884 | A |
| 25 | YA | 1888 | G |
| 25 | YA | 1889 | A |
| 25 | YA | 1903 | G |
| 25 | YA | 1906 | G |
| 25 | YA | 1919 | A |
| 25 | YA | 1929 | G |
| 25 | YA | 1930 | G |
| 25 | YA | 1931 | U |
| 25 | YA | 1936 | A |
| 25 | YA | 1939 | U |
| 25 | YA | 1955 | U |
| 25 | YA | 1960 | A |
| 25 | YA | 1963 | U |
| 25 | YA | 1965 | C |
| 25 | YA | 1967 | C |
| 25 | YA | 1969 | A |
| 25 | YA | 1970 | A |
| 25 | YA | 1971 | A |
| 25 | YA | 1972 | A |
| 25 | YA | 1982 | C |
| 25 | YA | 1992 | G |
| 25 | YA | 1993 | U |
| 25 | YA | 2004 | G |
| 25 | YA | 2020 | A |
| 25 | YA | 2021 | C |
| 25 | YA | 2023 | G |
| 25 | YA | 2031 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 2033 | A |
| 25 | YA | 2043 | C |
| 25 | YA | 2055 | C |
| 25 | YA | 2056 | G |
| 25 | YA | 2059 | A |
| 25 | YA | 2060 | A |
| 25 | YA | 2061 | G |
| 25 | YA | 2062 | A |
| 25 | YA | 2069 | G |
| 25 | YA | 2070 | G |
| 25 | YA | 2089 | U |
| 25 | YA | 2092 | U |
| 25 | YA | 2093 | G |
| 25 | YA | 2111 | C |
| 25 | YA | 2113 | U |
| 25 | YA | 2114 | A |
| 25 | YA | 2115 | G |
| 25 | YA | 2116 | G |
| 25 | YA | 2119 | A |
| 25 | YA | 2120 | G |
| 25 | YA | 2126 | A |
| 25 | YA | 2127 | G |
| 25 | YA | 2128 | C |
| 25 | YA | 2131 | G |
| 25 | YA | 2132 | U |
| 25 | YA | 2133 | G |
| 25 | YA | 2136 | C |
| 25 | YA | 2146 | C |
| 25 | YA | 2147 | G |
| 25 | YA | 2148 | G |
| 25 | YA | 2158 | A |
| 25 | YA | 2166 | G |
| 25 | YA | 2168 | G |
| 25 | YA | 2169 | A |
| 25 | YA | 2173 | A |
| 25 | YA | 2190 | G |
| 25 | YA | 2192 | G |
| 25 | YA | 2210 | G |
| 25 | YA | 2211 | G |
| 25 | YA | 2212 | A |
| 25 | YA | 2213 | U |
| 25 | YA | 2215 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 2225 | A |
| 25 | YA | 2238 | G |
| 25 | YA | 2239 | G |
| 25 | YA | 2243 | U |
| 25 | YA | 2266 | A |
| 25 | YA | 2275 | C |
| 25 | YA | 2278 | A |
| 25 | YA | 2280 | G |
| 25 | YA | 2283 | C |
| 25 | YA | 2287 | A |
| 25 | YA | 2288 | A |
| 25 | YA | 2307 | G |
| 25 | YA | 2308 | G |
| 25 | YA | 2309 | A |
| 25 | YA | 2311 | A |
| 25 | YA | 2312 | U |
| 25 | YA | 2319 | G |
| 25 | YA | 2320 | A |
| 25 | YA | 2325 | G |
| 25 | YA | 2335 | A |
| 25 | YA | 2342 | C |
| 25 | YA | 2345 | G |
| 25 | YA | 2346 | A |
| 25 | YA | 2347 | C |
| 25 | YA | 2350 | C |
| 25 | YA | 2383 | G |
| 25 | YA | 2385 | C |
| 25 | YA | 2392 | A |
| 25 | YA | 2394 | C |
| 25 | YA | 2402 | C |
| 25 | YA | 2403 | C |
| 25 | YA | 2406 | U |
| 25 | YA | 2423 | U |
| 25 | YA | 2424 | C |
| 25 | YA | 2425 | A |
| 25 | YA | 2427 | C |
| 25 | YA | 2428 | G |
| 25 | YA | 2429 | G |
| 25 | YA | 2430 | A |
| 25 | YA | 2434 | A |
| 25 | YA | 2435 | A |
| 25 | YA | 2439 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | YA | 2440 | C |
| 25 | YA | 2441 | C |
| 25 | YA | 2448 | A |
| 25 | YA | 2469 | A |
| 25 | YA | 2470 | G |
| 25 | YA | 2471 | C |
| 25 | YA | 2475 | C |
| 25 | YA | 2476 | A |
| 25 | YA | 2482 | G |
| 25 | YA | 2494 | G |
| 25 | YA | 2502 | G |
| 25 | YA | 2504 | U |
| 25 | YA | 2505 | G |
| 25 | YA | 2518 | A |
| 25 | YA | 2520 | C |
| 25 | YA | 2524 | G |
| 25 | YA | 2527 | C |
| 25 | YA | 2529 | G |
| 25 | YA | 2540 | C |
| 25 | YA | 2542 | A |
| 25 | YA | 2554 | U |
| 25 | YA | 2558 | C |
| 25 | YA | 2567 | G |
| 25 | YA | 2573 | C |
| 25 | YA | 2574 | G |
| 25 | YA | 2578 | G |
| 25 | YA | 2599 | G |
| 25 | YA | 2602 | A |
| 25 | YA | 2609 | U |
| 25 | YA | 2611 | U |
| 25 | YA | 2612 | C |
| 25 | YA | 2629 | A |
| 25 | YA | 2632 | A |
| 25 | YA | 2642 | G |
| 25 | YA | 2646 | C |
| 25 | YA | 2665 | A |
| 25 | YA | 2673 | G |
| 25 | YA | 2682 | U |
| 25 | YA | 2689 | U |
| 25 | YA | 2702 | U |
| 25 | YA | 2707 | G |
| 25 | YA | 2712 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 25 | YA | 2712(A) | A |
| 25 | YA | 2713 | A |
| 25 | YA | 2714 | G |
| 25 | YA | 2726 | U |
| 25 | YA | 2733 | A |
| 25 | YA | 2741 | A |
| 25 | YA | 2742 | C |
| 25 | YA | 2743 | C |
| 25 | YA | 2744 | G |
| 25 | YA | 2745 | C |
| 25 | YA | 2748 | A |
| 25 | YA | 2751 | G |
| 25 | YA | 2754 | U |
| 25 | YA | 2755 | C |
| 25 | YA | 2756 | U |
| 25 | YA | 2758 | A |
| 25 | YA | 2759 | G |
| 25 | YA | 2761 | G |
| 25 | YA | 2765 | A |
| 25 | YA | 2777 | G |
| 25 | YA | 2778 | A |
| 25 | YA | 2779 | U |
| 25 | YA | 2780 | G |
| 25 | YA | 2789 | C |
| 25 | YA | 2790 | A |
| 25 | YA | 2791 | C |
| 25 | YA | 2794 | C |
| 25 | YA | 2797 | U |
| 25 | YA | 2799 | A |
| 25 | YA | 2807 | G |
| 25 | YA | 2818 | G |
| 25 | YA | 2820 | A |
| 25 | YA | 2821 | A |
| 25 | YA | 2830 | G |
| 25 | YA | 2833 | G |
| 25 | YA | 2834 | G |
| 25 | YA | 2835 | A |
| 25 | YA | 2867 | G |
| 25 | YA | 2868 | A |
| 25 | YA | 2872 | G |
| 25 | YA | 2873 | A |
| 25 | YA | 2880 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | YA | 2891 | G |
| 25 | YA | 2892 | A |
| 25 | YA | 2893 | G |
| 25 | YA | 2894 | G |
| 26 | YB | 8 | U |
| 26 | YB | 13 | A |
| 26 | YB | 15 | A |
| 26 | YB | 16 | G |
| 26 | YB | 22 | U |
| 26 | YB | 25 | A |
| 26 | YB | 32 | C |
| 26 | YB | 41 | U |
| 26 | YB | 42 | C |
| 26 | YB | 45 | A |
| 26 | YB | 56 | G |
| 26 | YB | 66 | A |
| 26 | YB | 67 | G |
| 26 | YB | 73 | A |
| 26 | YB | 81 | G |
| 26 | YB | 82 | G |
| 26 | YB | 89 | G |
| 26 | YB | 90 | C |
| 26 | YB | 109 | G |

All (178) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | QA | 64 | G |
| 1 | QA | 115 | G |
| 1 | QA | 119 | A |
| 1 | QA | 181 | G |
| 1 | QA | 243 | A |
| 1 | QA | 250 | A |
| 1 | QA | 266 | G |
| 1 | QA | 328 | C |
| 1 | QA | 410 | G |
| 1 | QA | 412 | A |
| 1 | QA | 481 | G |
| 1 | QA | 484 | G |
| 1 | QA | 485 | G |
| 1 | QA | 509 | A |
| 1 | QA | 533 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | QA | 687 | A |
| 1 | QA | 703 | G |
| 1 | QA | 753 | A |
| 1 | QA | 792 | A |
| 1 | QA | 812 | C |
| 1 | QA | 913 | A |
| 1 | QA | 992 | U |
| 1 | QA | 1027 | C |
| 1 | QA | 1065 | U |
| 1 | QA | 1200 | C |
| 1 | QA | 1201 | A |
| 1 | QA | 1285 | A |
| 1 | QA | 1297 | C |
| 1 | QA | 1301 | U |
| 1 | QA | 1336 | C |
| 1 | QA | 1346 | A |
| 1 | QA | 1347 | G |
| 1 | QA | 1498 | U |
| 1 | QA | 1528 | U |
| 22 | QV | 20 | G |
| 22 | QV | 35 | C |
| 22 | QV | 53 | G |
| 22 | QW | 8 | U |
| 22 | QW | 59 | A |
| 25 | RA | 99 | U |
| 25 | RA | 102 | G |
| 25 | RA | 221 | A |
| 25 | RA | 229 | A |
| 25 | RA | 242 | G |
| 25 | RA | 271(B) | G |
| 25 | RA | 345 | A |
| 25 | RA | 372 | G |
| 25 | RA | 404 | C |
| 25 | RA | 503 | A |
| 25 | RA | 512 | G |
| 25 | RA | 587 | C |
| 25 | RA | 637 | A |
| 25 | RA | 752 | A |
| 25 | RA | 846 | C |
| 25 | RA | 856 | C |
| 25 | RA | 974(A) | C |
| 25 | RA | 1012 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 25 | RA | 1022 | G |
| 25 | RA | 1026 | U |
| 25 | RA | 1032 | A |
| 25 | RA | 1045 | A |
| 25 | RA | 1078 | U |
| 25 | RA | 1085 | A |
| 25 | RA | 1178 | C |
| 25 | RA | 1204 | A |
| 25 | RA | 1210 | A |
| 25 | RA | 1312 | U |
| 25 | RA | 1427 | A |
| 25 | RA | 1558 | A |
| 25 | RA | 1653 | G |
| 25 | RA | 1694 | C |
| 25 | RA | 1799 | G |
| 25 | RA | 1819 | A |
| 25 | RA | 1930 | G |
| 25 | RA | 1992 | G |
| 25 | RA | 2060 | A |
| 25 | RA | 2126 | A |
| 25 | RA | 2405 | G |
| 25 | RA | 2439 | A |
| 25 | RA | 2481 | G |
| 25 | RA | 2566 | A |
| 25 | RA | 2610 | C |
| 25 | RA | 2689 | U |
| 25 | RA | 2712 | U |
| 25 | RA | 2776 | A |
| 25 | RA | 2832 | U |
| 26 | RB | 66 | A |
| 1 | XA | 5 | U |
| 1 | XA | 60 | A |
| 1 | XA | 64 | G |
| 1 | XA | 78 | G |
| 1 | XA | 89 | U |
| 1 | XA | 115 | G |
| 1 | XA | 243 | A |
| 1 | XA | 244 | U |
| 1 | XA | 250 | A |
| 1 | XA | 266 | G |
| 1 | XA | 328 | C |
| 1 | XA | 345 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | XA | 352 | C |
| 1 | XA | 410 | G |
| 1 | XA | 412 | A |
| 1 | XA | 429 | U |
| 1 | XA | 481 | G |
| 1 | XA | 484 | G |
| 1 | XA | 485 | G |
| 1 | XA | 509 | A |
| 1 | XA | 560 | U |
| 1 | XA | 687 | A |
| 1 | XA | 703 | G |
| 1 | XA | 753 | A |
| 1 | XA | 812 | C |
| 1 | XA | 913 | A |
| 1 | XA | 991 | U |
| 1 | XA | 992 | U |
| 1 | XA | 1027 | C |
| 1 | XA | 1065 | U |
| 1 | XA | 1200 | C |
| 1 | XA | 1285 | A |
| 1 | XA | 1297 | C |
| 1 | XA | 1301 | U |
| 1 | XA | 1336 | C |
| 1 | XA | 1446 | A |
| 1 | XA | 1498 | U |
| 22 | XV | 20 | G |
| 22 | XV | 35 | C |
| 22 | XV | 53 | G |
| 22 | XW | 8 | U |
| 22 | XW | 59 | A |
| 25 | YA | 99 | U |
| 25 | YA | 195 | A |
| 25 | YA | 221 | A |
| 25 | YA | 222 | A |
| 25 | YA | 229 | A |
| 25 | YA | 241 | A |
| 25 | YA | 242 | G |
| 25 | YA | 271(B) | G |
| 25 | YA | 278 | A |
| 25 | YA | 372 | G |
| 25 | YA | 404 | C |
| 25 | YA | 503 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 25 | YA | 587 | C |
| 25 | YA | 637 | A |
| 25 | YA | 752 | A |
| 25 | YA | 846 | C |
| 25 | YA | 856 | C |
| 25 | YA | 859 | G |
| 25 | YA | 974(A) | C |
| 25 | YA | 1012 | U |
| 25 | YA | 1022 | G |
| 25 | YA | 1026 | U |
| 25 | YA | 1045 | A |
| 25 | YA | 1078 | U |
| 25 | YA | 1085 | A |
| 25 | YA | 1109 | C |
| 25 | YA | 1178 | C |
| 25 | YA | 1210 | A |
| 25 | YA | 1379 | A |
| 25 | YA | 1427 | A |
| 25 | YA | 1558 | A |
| 25 | YA | 1653 | G |
| 25 | YA | 1694 | C |
| 25 | YA | 1698 | A |
| 25 | YA | 1799 | G |
| 25 | YA | 1819 | A |
| 25 | YA | 1930 | G |
| 25 | YA | 1992 | G |
| 25 | YA | 2126 | A |
| 25 | YA | 2212 | A |
| 25 | YA | 2439 | A |
| 25 | YA | 2566 | A |
| 25 | YA | 2610 | C |
| 25 | YA | 2681 | C |
| 25 | YA | 2712 | U |
| 25 | YA | 2743 | C |
| 25 | YA | 2776 | A |
| 25 | YA | 2867 | G |
| 26 | YB | 66 | A |

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1301 ligands modelled in this entry, 1299 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 | $\# Z > 2$ |
| 57 | SF4 | XD | 301 | 4 | 0,12,12 | 0.00 | - | - | | |
| 57 | SF4 | QD | 301 | 4 | 0,12,12 | 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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 57 | SF4 | XD | 301 | 4 | - | - | 0/6/5/5 |
| 57 | SF4 | QD | 301 | 4 | - | - | 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.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 57 | QD | 301 | SF4 | 1 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.