



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:55 PM GMT

PDB ID : 2QBC
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin. This file contains the 50S subunit of the second 70S ribosome, with gentamicin bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-16
Resolution : 3.54 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

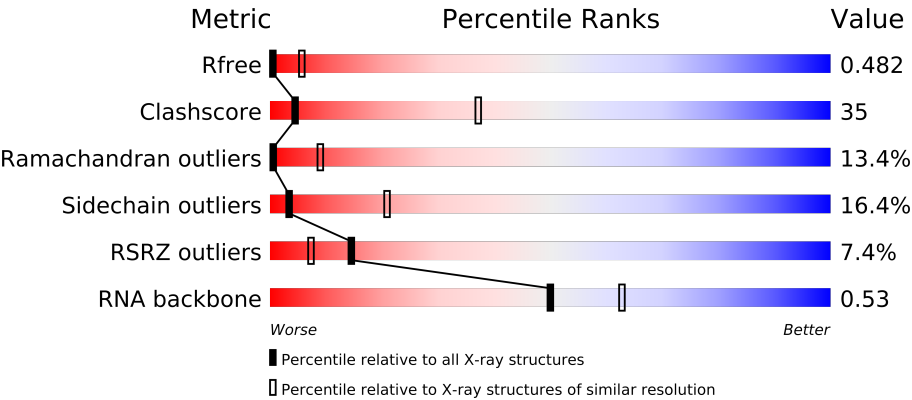
The following versions of software and data (see [references](#)) were used in the production of this report:

| | | |
|--------------------------------|---|--------------------------|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.15 2013 |
| Xtriage (Phenix) | : | dev-1323 |
| EDS | : | stable22639 |
| Percentile statistics | : | 21963 |
| Refmac | : | 5.8.0049 |
| CCP4 | : | 6.3.0 (Settle) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable22683 |

1 Overall quality at a glance

The reported resolution of this entry is 3.54 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)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1270 (3.78-3.30) |
| Clashscore | 79885 | 1033 (3.70-3.38) |
| Ramachandran outliers | 78287 | 1067 (3.72-3.36) |
| Sidechain outliers | 78261 | 1067 (3.72-3.36) |
| RSRZ outliers | 66119 | 1270 (3.78-3.30) |
| RNA backbone | 1838 | 1011 (4.30-2.76) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 120 | |
| 2 | B | 2904 | |
| 3 | I | 141 | |
| 4 | C | 272 | |
| 5 | D | 209 | |
| 6 | K | 123 | |
| 7 | P | 114 | |
| 8 | E | 201 | |
| 9 | Y | 58 | |
| 10 | 0 | 56 | |
| 11 | 4 | 38 | |
| 12 | 1 | 54 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 13 | 3 | 64 | |
| 14 | V | 94 | |
| 15 | 2 | 46 | |
| 16 | L | 144 | |
| 17 | M | 136 | |
| 18 | X | 63 | |
| 19 | H | 149 | |
| 20 | J | 142 | |
| 21 | N | 127 | |
| 22 | O | 117 | |
| 23 | Q | 117 | |
| 24 | S | 110 | |
| 25 | U | 103 | |
| 26 | F | 178 | |
| 27 | G | 176 | |
| 28 | R | 103 | |
| 29 | T | 100 | |
| 30 | Z | 78 | |
| 31 | W | 84 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 32 | MG | B | 3165 | - | X |
| 32 | MG | B | 3201 | - | X |
| 32 | MG | B | 3207 | - | X |
| 32 | MG | B | 3262 | - | X |
| 32 | MG | B | 3279 | - | X |
| 32 | MG | B | 3337 | - | X |
| 32 | MG | B | 3452 | - | X |
| 32 | MG | B | 3515 | - | X |
| 34 | LLL | B | 3619 | - | X |

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 90294 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 1 | A | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |

- Molecule 2 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 2 | B | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | I | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | C | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | D | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | K | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | P | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | E | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | Y | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | 0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | 4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 12 | 1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 13 | 3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | V | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 15 | 2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | L | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | M | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18 | X | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | H | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | J | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | N | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 22 | O | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |

- Molecule 23 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 23 | Q | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |

- Molecule 24 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | S | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 25 | U | 102 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |

- Molecule 26 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | F | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | G | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | R | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | T | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | Z | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | W | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |

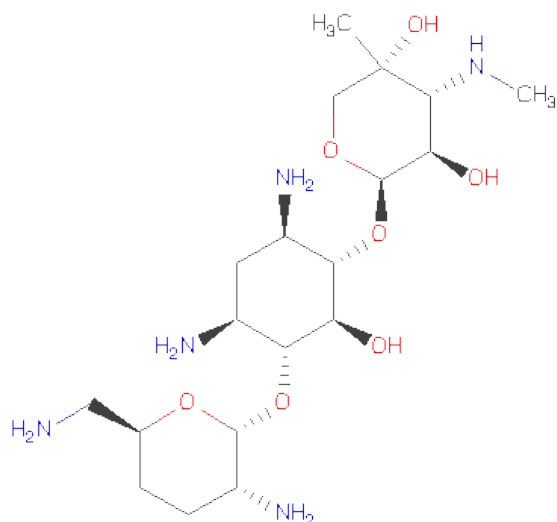
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 32 | B | 111 | Total | Mg | 0 | 0 |
| | | | 111 | 111 | | |

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33 | 4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 34 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 34 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

- Molecule 35 is water.

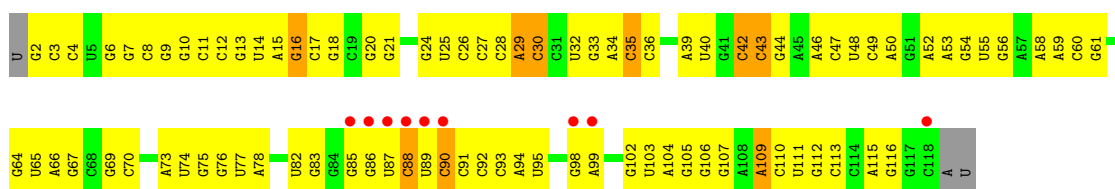
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 35 | B | 502 | Total | O | 0 | 0 |
| | | | 502 | 502 | | |
| 35 | C | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 35 | E | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 35 | L | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

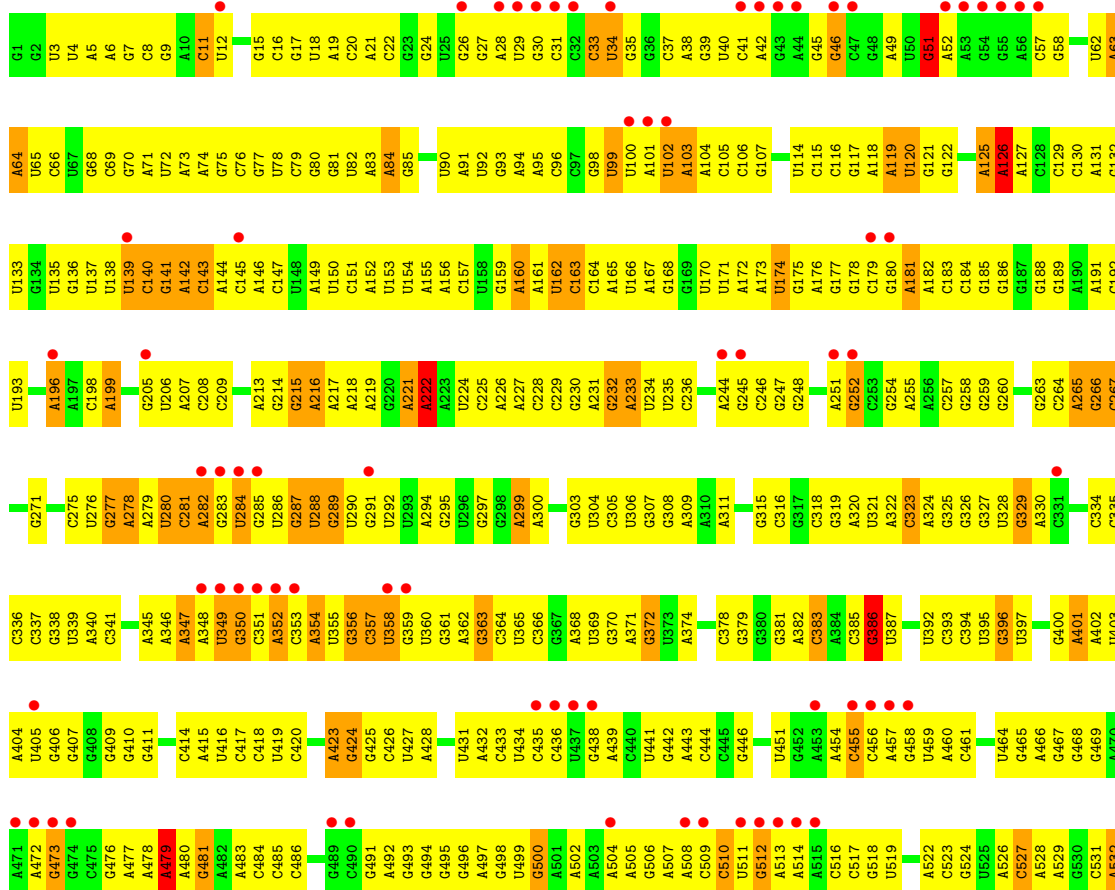
• Molecule 1: 5S rRNA

Chain A: 



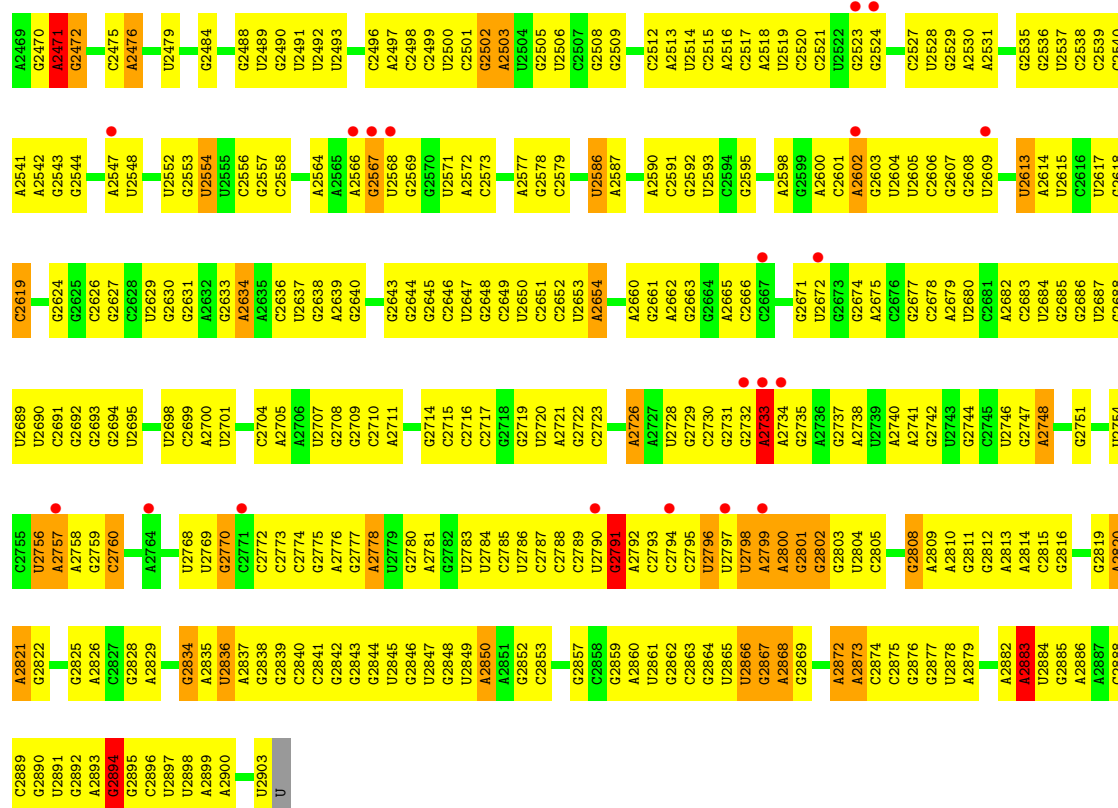
• Molecule 2: 23S rRNA

Chain B: 



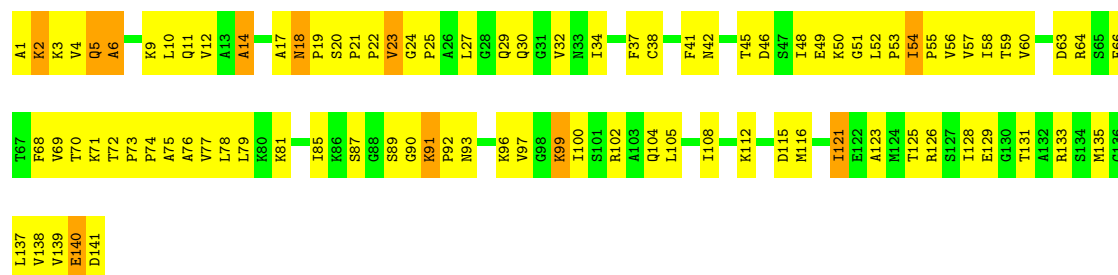
| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|
| U1466 | A1403 | G1337 | A1269 | U1203 | C1140 | A996 | A933 | U870 | G805 | G726 | A661 | G597 | G533 |
| A1469 | C1404 | G1338 | G1270 | A1204 | U1141 | G997 | U934 | U871 | C806 | A727 | G664 | U596 | U534 |
| U1470 | U1405 | G1339 | G1271 | A1205 | A1142 | C998 | C935 | U872 | U807 | U728 | U665 | A599 | G535 |
| G1471 | U1406 | U1340 | A1272 | G1206 | A1143 | U999 | A936 | G873 | G808 | G729 | U666 | G600 | G536 |
| U1475 | G1407 | G1341 | U1273 | C1207 | A1144 | A1000 | C937 | G874 | G809 | A730 | A666 | C601 | G537 |
| U1476 | G1408 | G1342 | A1274 | C1208 | U1145 | A1001 | G938 | G875 | U810 | G731 | U667 | A602 | A538 |
| U1477 | U1409 | U1343 | A1275 | U1209 | C1146 | G1002 | A941 | C876 | U811 | C736 | A668 | G539 | G539 |
| U1478 | G1410 | G1344 | A1276 | G1210 | A1147 | A1009 | G942 | A877 | C812 | G737 | G669 | C540 | C540 |
| U1479 | U1411 | G1345 | G1277 | G1212 | U1148 | A1010 | A943 | A878 | U813 | G738 | A670 | G605 | A541 |
| G1480 | U1412 | U1346 | G1280 | G1215 | C1149 | G1011 | U946 | G | C814 | U739 | C672 | G605 | C542 |
| G1482 | G1416 | G1347 | U1281 | G1216 | A1151 | U1012 | C947 | G | C815 | G740 | C673 | A608 | C544 |
| G1483 | C1417 | A1348 | U1282 | C1217 | A1152 | C1013 | C948 | G | C816 | U741 | C674 | A609 | U545 |
| U1484 | U1418 | A1349 | G1283 | U1217 | C1153 | A1014 | C949 | G | C817 | A742 | A675 | G611 | U546 |
| U1485 | G1419 | U1350 | A1284 | G1218 | U1154 | U1015 | G949 | U | C818 | A743 | A676 | G612 | A547 |
| U1486 | A1420 | G1351 | A1285 | U1219 | A1155 | G1016 | C950 | C | A820 | U744 | A677 | A613 | G548 |
| U1487 | G1421 | G1352 | A1286 | G1220 | A1156 | U1017 | C951 | A | A821 | G745 | C678 | A614 | U549 |
| U1488 | U1422 | C1357 | A1287 | C1221 | U1159 | U1018 | G952 | U | G822 | U746 | C679 | U615 | C550 |
| G1489 | G1425 | G1358 | G1288 | U1222 | U1160 | U1019 | G953 | C | C823 | U747 | C680 | A616 | G551 |
| A1490 | G1426 | U1359 | U1223 | G1223 | C1161 | A1020 | U954 | C | U824 | G748 | G682 | G617 | U554 |
| G1491 | A1427 | G1360 | U1224 | U1224 | G1162 | A1021 | U955 | A753 | A825 | A749 | U683 | G620 | G555 |
| G1492 | G1428 | G1361 | G1228 | G1228 | U1163 | U1022 | C956 | U754 | U826 | U755 | U686 | A621 | A556 |
| C1493 | U1429 | U1362 | A1230 | G1229 | G1164 | G1023 | C957 | U756 | U827 | U757 | C687 | C623 | C557 |
| A1494 | G1430 | U1365 | A1231 | U1231 | U1165 | G1024 | U958 | A758 | U828 | G759 | U688 | C624 | G559 |
| A1496 | G1431 | G1366 | U1232 | U1232 | G1166 | U1025 | A959 | C | U829 | G759 | A689 | G625 | C560 |
| G1501 | G1432 | U1368 | G1296 | G1235 | U1167 | A1026 | A960 | C | G831 | G765 | U689 | A626 | G561 |
| A1502 | A1433 | G1369 | C1297 | G1236 | U1168 | A1027 | A961 | A | U832 | U766 | C690 | A627 | U562 |
| A1503 | U1434 | U1370 | G1298 | U1237 | G1169 | U1028 | C962 | C | U833 | U767 | C691 | C628 | A563 |
| A1504 | G1437 | G1371 | G1299 | G1238 | C1170 | C1030 | C965 | A899 | G834 | U768 | A693 | G629 | C564 |
| A1505 | U1438 | U1372 | G1300 | G1239 | G1171 | G1031 | U966 | U | C835 | U769 | U694 | C630 | C565 |
| U1506 | A1439 | A1373 | U1301 | U1240 | C1172 | A1032 | U967 | C903 | C836 | U770 | G695 | A631 | U567 |
| C1507 | U1440 | G1374 | G1302 | A1241 | U1173 | U1033 | C968 | G904 | U837 | G771 | G696 | A632 | G570 |
| A1508 | G1441 | U1375 | C1303 | C1242 | U1174 | G1037 | U969 | U904 | C838 | U772 | C697 | A633 | U571 |
| A1509 | U1442 | G1376 | A1304 | C1243 | U1175 | G1038 | U970 | A905 | C840 | U773 | C698 | C634 | U572 |
| U1510 | U1443 | U1377 | U1307 | C1244 | U1176 | A1039 | A971 | U906 | U841 | U774 | G700 | C635 | A573 |
| G1511 | G1444 | U1378 | A1308 | G1245 | G1177 | A1040 | A972 | G907 | U842 | G775 | G701 | A637 | U573 |
| U1512 | U1445 | G1380 | G1309 | U1246 | C1178 | U1041 | A973 | C908 | A845 | G776 | U702 | G638 | U574 |
| U1513 | G1446 | U1381 | U1247 | A1247 | U1180 | G1042 | A974 | A909 | U846 | G777 | U703 | U639 | A575 |
| G1514 | C1447 | A1382 | G1310 | U1248 | U1181 | U1043 | A975 | A910 | U847 | G778 | G704 | C640 | U576 |
| A1515 | U1448 | U1383 | G1311 | U1249 | U1182 | C1044 | G976 | C912 | C848 | U779 | A705 | U641 | G577 |
| G1516 | G1449 | A1384 | U1312 | C1250 | U1183 | U1045 | A977 | U913 | U850 | G780 | U706 | U642 | G578 |
| G1517 | U1450 | U1385 | C1315 | G1251 | G1187 | A1046 | A980 | A917 | C851 | U781 | G707 | A643 | G579 |
| C1518 | C1451 | G1386 | U1316 | G1252 | U1188 | U1047 | A981 | A918 | U852 | U782 | U708 | A644 | U580 |
| A1524 | U1452 | A1387 | G1317 | A1253 | U1189 | G1047 | C982 | U919 | C853 | A783 | U709 | C645 | C581 |
| A1525 | A1453 | U1388 | U1318 | U1254 | G1190 | G1048 | C983 | A920 | C854 | G784 | U710 | U646 | A582 |
| G1526 | G1454 | G1389 | C1319 | G1255 | G1191 | U1050 | A984 | C921 | G855 | U785 | G711 | G583 | G583 |
| G1527 | U1455 | U1391 | C1320 | C1256 | G1192 | C1052 | C985 | C922 | G856 | U786 | G712 | G649 | C587 |
| U1528 | G1456 | A1392 | A1321 | U1257 | G1193 | C1053 | C986 | G923 | C857 | A788 | G713 | C650 | U588 |
| U1529 | U1457 | U1393 | C1322 | U1258 | U1194 | A1054 | C987 | G924 | G858 | U789 | C717 | U653 | U589 |
| G1530 | U1458 | A1394 | U1323 | A1259 | G1195 | G1055 | A988 | A925 | C859 | A790 | C718 | A654 | A590 |
| C1531 | U1459 | U1395 | G1324 | C1261 | U1196 | U1060 | G989 | G926 | A863 | C795 | C719 | A655 | U591 |
| A1532 | U1460 | U1396 | U1325 | U1262 | G1197 | U1061 | A990 | A927 | A864 | C796 | U720 | G656 | A592 |
| U1533 | U1461 | U1397 | U1326 | U1263 | U1198 | G1062 | C991 | A928 | C865 | G797 | A721 | U657 | U593 |
| U1534 | C1462 | U1400 | G1334 | U1266 | U1199 | G1063 | C992 | U929 | A866 | G798 | A722 | U658 | C594 |
| A1535 | G1463 | G1401 | C1335 | U1267 | C1200 | C1064 | C993 | G930 | U931 | U803 | C723 | G659 | U595 |
| C1536 | U1464 | U1402 | A1336 | A1268 | G1202 | U1065 | C995 | U932 | C869 | A804 | | C660 | U596 |

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| G2405 | A2406 | A2407 | U2408 | G2409 | G2410 | A2411 | A2412 | G2413 | G2414 | G2415 | G2416 | G2417 | A2418 | U2419 | G2420 | G2421 | G2422 | G2423 | G2424 | A2425 | A2426 | C2427 | G2428 | A2429 | A2430 | A2434 | A2435 | U2438 | A2439 | U2440 | U2441 | C2442 | G2443 | G2444 | G2445 | G2446 | G2447 | A2448 | U2449 | A2450 | A2451 | G2454 | G2455 | G2456 | U2457 | G2458 | A2459 | U2460 | A2461 | C2462 | G2463 | G2464 | G2465 | C2466 | C2467 | A2468 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C2339 | A2340 | G2341 | G2342 | U2343 | U2344 | G2345 | G2346 | C2347 | U2348 | G2349 | A2352 | G2353 | G2354 | G2355 | U2356 | G2357 | G2358 | G2359 | G2360 | G2361 | A2297 | A2298 | U2299 | G2363 | G2364 | G2365 | A2366 | G2367 | A2368 | G2369 | G2370 | G2371 | C2374 | G2375 | A2376 | A2377 | A2378 | G2379 | G2383 | U2384 | U2385 | U2386 | U2387 | A2388 | G2389 | U2390 | U2393 | G2394 | G2395 | G2396 | G2397 | U2398 | G2399 | G2400 | U2401 | U2402 | U2403 | U2404 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A2274 | C2275 | G2276 | G2279 | G2280 | A2281 | G2282 | G2283 | C2284 | A2285 | G2286 | A2287 | A2288 | U2291 | U2292 | G2293 | G2294 | G2295 | U2296 | A2297 | A2298 | U2299 | G2300 | C2301 | U2302 | A2303 | G2304 | U2305 | G2306 | G2307 | G2308 | A2309 | G2310 | A2311 | U2312 | A2313 | A2314 | G2315 | G2316 | U2320 | U2321 | A2322 | G2323 | U2324 | G2325 | U2328 | U2329 | G2330 | G2331 | G2332 | A2333 | U2334 | A2335 | A2336 | G2337 | G2338 | G2339 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A2212 | U2213 | C2214 | C2215 | G2216 | G2217 | G2218 | U2219 | U2220 | G2221 | G2222 | G2223 | G2224 | A2225 | G2226 | A2227 | G2228 | U2229 | G2230 | U2231 | U2232 | U2233 | G2234 | U2235 | G2236 | G2237 | G2238 | G2239 | U2240 | A2241 | G2242 | U2243 | U2244 | G2245 | G2246 | A2247 | C2248 | U2249 | U2250 | G2251 | G2255 | G2256 | C2257 | U2258 | U2259 | G2260 | C2261 | U2262 | C2263 | C2264 | U2265 | A2266 | A2267 | A2268 | U2269 | G2270 | U2271 | U2272 | A2273 | G2274 | G2275 | G2276 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C2150 | U2151 | G2152 | C2153 | A2154 | U2155 | G2156 | G2157 | A | G | C | C | G | A | C | C | C | U | G | A | A | U | G | A | C | C | C | A | C | C | C2179 | U2180 | U2181 | U2182 | A2183 | U2184 | U2185 | U2186 | U2187 | U2188 | U2189 | A2190 | A2191 | U2192 | G2193 | U2194 | U2195 | C2196 | U2197 | A2198 | A2199 | C2200 | U2203 | G2204 | C2207 | C2208 | G2209 | U2210 | A2211 | U2212 | A2213 | A2214 | A2215 | A2216 | A2217 | A2218 | A2219 | A2220 | A2221 | A2222 | A2223 | A2224 | A2225 | A2226 | A2227 | A2228 | A2229 | A2230 | A2231 | A2232 | A2233 | A2234 | A2235 | A2236 | A2237 | A2238 | A2239 | A2240 | A2241 | A2242 | A2243 | A2244 | A2245 | A2246 | A2247 | A2248 | A2249 | A2250 | A2251 | A2252 | A2253 | A2254 | A2255 | A2256 | A2257 | A2258 | A2259 | A2260 | A2261 | A2262 | A2263 | A2264 | A2265 | A2266 | A2267 | A2268 | A2269 | A2270 | A2271 | A2272 | A2273 | A2274 | A2275 | A2276 | A2277 | A2278 | A2279 | A2280 | A2281 | A2282 | A2283 | A2284 | A2285 | A2286 | A2287 | A2288 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| A2539 | A2540 | A2541 | A2542 | A2543 | A2544 | A2545 | A2546 | A2547 | A2548 | A2549 | A2550 | A2551 | A2552 | A2553 | A2554 | A2555 | A2556 | A2557 | A2558 | A2559 | A2560 | A2561 | A2562 | A2563 | A2564 | A2565 | A2566 | A2567 | A2568 | A2569 | A2570 | A2571 | A2572 | A2573 | A2574 | A2575 | A2576 | A2577 | A2578 | A2579 | A2580 | A2581 | A2582 | A2583 | A2584 | A2585 | A2586 | A2587 | A2588 | A2589 | A2590 | A2591 | A2592 | A2593 | A2594 | A2595 | A2596 | A2597 | A2598 | A2599 | A2600 | A2601 | A2602 | A2603 | A2604 | A2605 | A2606 | A2607 | A2608 | A2609 | A2610 | A2611 | A2612 | A2613 | A2614 | A2615 | A2616 | A2617 | A2618 | A2619 | A2620 | A2621 | A2622 | A2623 | A2624 | A2625 | A2626 | A2627 | A2628 | A2629 | A2630 | A2631 | A2632 | A2633 | A2634 | A2635 | A2636 | A2637 | A2638 | A2639 | A2640 | A2641 | A2642 | A2643 | A2644 | A2645 | A2646 | A2647 | A2648 | A2649 | A2650 | A2651 | A2652 | A2653 | A2654 | A2655 | A2656 | A2657 | A2658 | A2659 | A2660 | A2661 | A2662 | A2663 | A2664 | A2665 | A2666 | A2667 | A2668 | A2669 | A2670 | A2671 | A2672 | A2673 | A2674 | A2675 | A2676 | A2677 | A2678 | A2679 | A2680 | A2681 | A2682 | A2683 | A2684 | A2685 | A2686 | A2687 | A2688 | A2689 | A2690 | A2691 | A2692 | A2693 | A2694 | A2695 | A2696 | A2697 | A2698 | A2699 | A2700 | A2701 | A2702 | A2703 | A2704 | A2705 | A2706 | A2707 | A2708 | A2709 | A2710 | A2711 | A2712 | A2713 | A2714 | A2715 | A2716 | A2717 | A2718 | A2719 | A2720 | A2721 | A2722 | A2723 | A2724 | A2725 | A2726 | A2727 | A2728 | A2729 | A2730 | A2731 | A2732 | A2733 | A2734 | A2735 | A2736 | A2737 | A2738 | A2739 | A2740 | A2741 | A2742 | A2743 | A2744 | A2745 | A2746 | A2747 | A2748 | A2749 | A2750 | A2751 | A2752 | A2753 | A2754 | A2755 | A2756 | A2757 | A2758 | A2759 | A2760 | A2761 | A2762 | A2763 | A2764 | A2765 | A2766 | A2767 | A2768 | A2769 | A2770 | A2771 | A2772 | A2773 | A2774 | A2775 | A2776 | A2777 | A2778 | A2779 | A2780 | A2781 | A2782 | A2783 | A2784 | A2785 | A2786 | A2787 | A2788 | A2789 | A2790 | A2791 | A2792 | A2793 | A2794 | A2795 | A2796 | A2797 | A2798 | A2799 | A2800 | A2801 | A2802 | A2803 | A2804 | A2805 | A2806 | A2807 | A2808 | A2809 | A2810 | A2811 | A2812 | A2813 | A2814 | A2815 | A2816 | A2817 | A2818 | A2819 | A2820 | A2821 | A2822 | A2823 | A2824 | A2825 | A2826 | A2827 | A2828 | A2829 | A2830 | A2831 | A2832 | A2833 | A2834 | A2835 | A2836 | A2837 | A2838 | A2839 | A2840 | A2841 | A2842 | A2843 | A2844 | A2845 | A2846 | A2847 | A2848 | A2849 | A2850 | A2851 | A2852 | A2853 | A2854 | A2855 | A2856 | A2857 | A2858 | A2859 | A2860 | A2861 | A2862 | A2863 | A2864 | A2865 | A2866 | A2867 | A2868 | A2869 | A2870 | A2871 | A2872 | A2873 | A2874 | A2875 | A2876 | A2877 | A2878 | A2879 | A2880 | A2881 | A2882 | A2883 | A2884 | A2885 | A2886 | A2887 | A2888 | A2889 | A2890 | A2891 | A2892 | A2893 | A2894 | A2895 | A2896 | A2897 | A2898 | A2899 | A2900 | A2901 | A2902 | A2903 | A2904 | A2905 | A2906 | A2907 | A2908 | A2909 | A2910 | A2911 | A2912 | A2913 | A2914 | A2915 | A2916 | A2917 | A2918 | A2919 | A2920 | A2921 | A2922 | A2923 | A2924 | A2925 | A2926 | A2927 | A2928 | A2929 | A2930 | A2931 | A2932 | A2933 | A2934 | A2935 | A2936 | A2937 | A2938 | A2939 | A2940 | A2941 | A2942 | A2943 | A2944 | A2945 | A2946 | A2947 | A2948 | A2949 | A2950 | A2951 | A2952 | A2953 | A2954 | A2955 | A2956 | A2957 | A2958 | A2959 | A2960 | A2961 | A2962 | A2963 | A2964 | A2965 | A2966 | A2967 | A2968 | A2969 | A2970 | A2971 | A2972 | A2973 | A2974 | A2975 | A2976 | A2977 | A2978 | A2979 | A2980 | A2981 | A2982 | A2983 | A2984 | A2985 | A2986 | A2987 | A2988 | A2989 | A2990 | A2991 | A2992 | A2993 | A2994 | A2995 | A2996 | A2997 | A2998 | A2999 | A3000 | A3001 | A3002 | A3003 | A3004 | A3005 | A3006 | A3007 | A3008 | A3009 | A3010 | A3011 | A3012 | A3013 | A3014 | A3015 | A3016 | A3017 | A3018 | A3019 | A3020 | A3021 | A3022 | A3023 | A3024 | A3025 | A3026 | A3027 | A3028 | A3029 | A3030 | A3031 | A3032 | A3033 | A3034 | A3035 | A3036 | A3037 | A3038 | A3039 | A3040 | A3041 | A3042 | A3043 | A3044 | A3045 | A3046 | A3047 | A3048 | A3049 | A3050 | A3051 | A3052 | A3053 | A3054 | A3055 | A3056 | A3057 | A3058 | A3059 | A3060 | A3061 | A3062 | A3063 | A3064 | A3065 | A3066 | A3067 | A3068 | A3069 | A3070 | A3071 | A3072 | A3073 | A3074 | A3075 | A3076 | A3077 | A3078 | A3079 | A3080 | A3081 | A3082 | A3083 | A3084 | A3085 | A3086 | A3087 | A3088 | A3089 | A3090 | A3091 | A3092 | A3093 | A3094 | A3095 | A3096 | A3097 | A3098 | A3099 | A3100 | A3101 | A3102 | A3103 | A3104 | A3105 | A3106 | A3107 | A3108 | A3109 | A3110 | A3111 | A3112 | A3113 | A3114 | A3115 | A3116 | A3117 | A3118 | A3119 | A3120 | A3121 | A3122 | A3123 | A3124 | A3125 | A3126 | A3127 | A3128 | A3129 | A3130 | A3131 | A3132 | A3133 | A3134 | A3135 | A3136 | A3137 | A3138 | A3139 | A3140 | A3141 | A3142 | A3143 | A3144 | A3145 | A3146 | A3147 | A3148 | A3149 | A3150 | A3151 | A3152 | A3153 | A3154 | A3155 | A3156 | A3157 | A3158 | A3159 | A3160 | A3161 | A3162 | A3163 | A3164 | A3165 | A3166 | A3167 | A3168 | A3169 | A3170 | A3171 | A3172 | A3173 | A3174 | A3175 | A3176 | A3177 | A3178 | A3179 | A3180 | A3181 | A3182 | A3183 | A3184 | A3185 | A3186 | A3187 | A3188 | A3189 | A3190 | A3191 | A3192 | A3193 | A3194 | A3195 | A3196 | A3197 | A3198 | A3199 | A3200 | A3201 | A3202 | A3203 | A3204 | A3205 | A3206 | A3207 | A3208 | A3209 | A3210 | A3211 | A3212 | A3213 | A3214 | A3215 | A3216 | A3217 | A3218 | A3219 | A3220 | A3221 | A3222 | A3223 | A3224 | A3225 | A3226 | A3227 | A3228 | A3229 | A3230 | A3231 | A3232 | A3233 | A3234 | A3235 | A3236 | A3237 | A3238 | A3239 | A3240 | A3241 | A3242 | A3243 | A3244 | A3245 | A3246 | A3247 | A3248 | A3249 | A3250 | A3251 | A3252 | A3253 | A3254 | A3255 | A3256 | A3257 | A3258 | A3259 | A3260 | A3261 | A3262 | A3263 | A3264 | A3265 | A3266 | A3267 | A3268 | A3269 | A3270 | A3271 | A3272 | A3273 | A3274 | A3275 | A3276 | A3277 | A3278 | A3279 | A3280 | A3281 | A3282 | A3283 | A3284 | A3285 | A3286 | A3287 | A3288 | A3289 | A3290 | A3291 | A3292 |



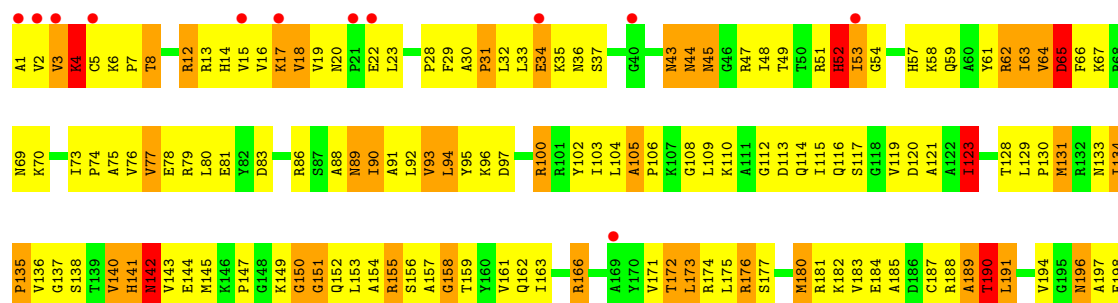
- Molecule 3: 50S ribosomal protein L11

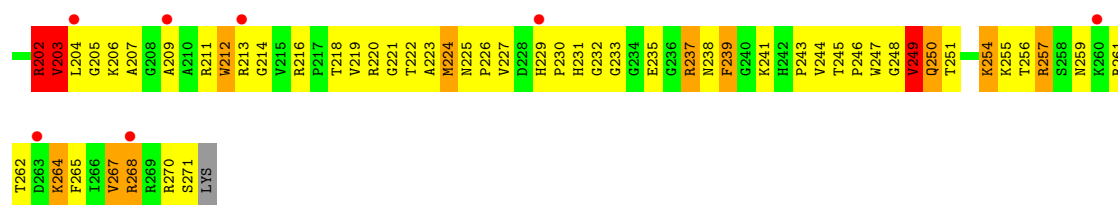
Chain I:



- Molecule 4: 50S ribosomal protein L2

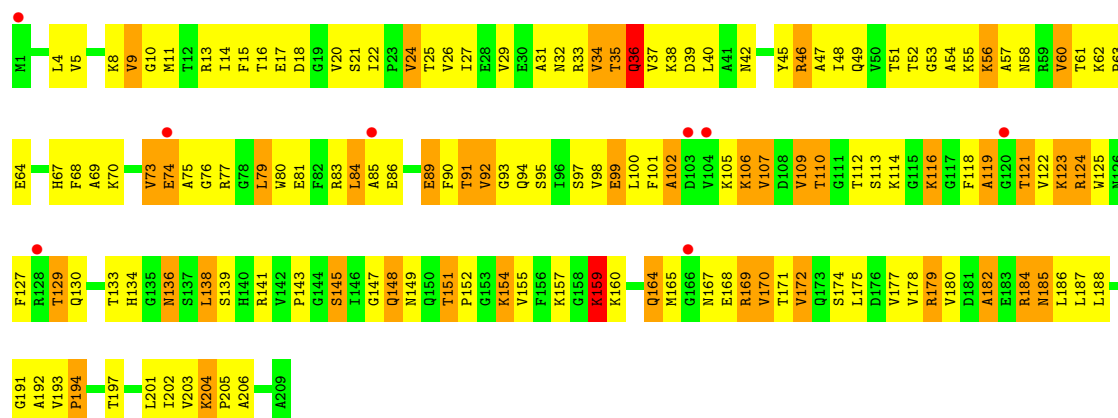
Chain C:





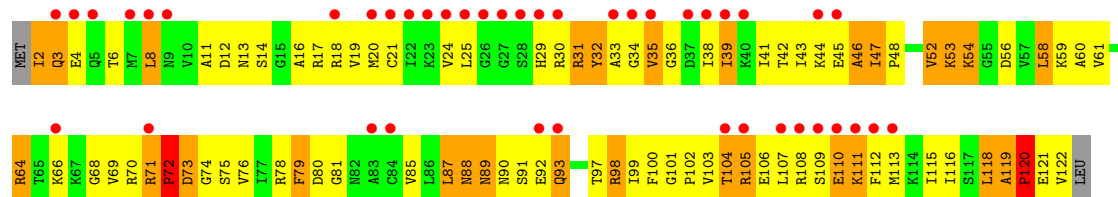
- Molecule 5: 50S ribosomal protein L3

Chain D:



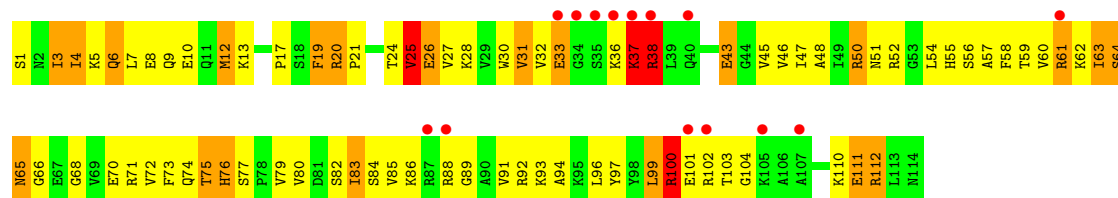
- Molecule 6: 50S ribosomal protein L14

Chain K:



- Molecule 7: 50S ribosomal protein L19

Chain P:



- Molecule 8: 50S ribosomal protein L4

Chain E: 





• Molecule 9: 50S ribosomal protein L30

Chain Y:



• Molecule 10: 50S ribosomal protein L32

Chain 0:



• Molecule 11: 50S ribosomal protein L36

Chain 4:



• Molecule 12: 50S ribosomal protein L33

Chain 1:



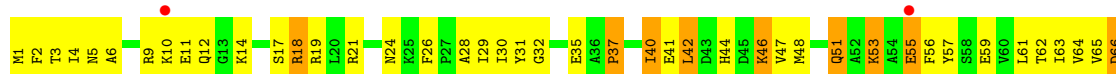
• Molecule 13: 50S ribosomal protein L35

Chain 3:



• Molecule 14: 50S ribosomal protein L25

Chain V:



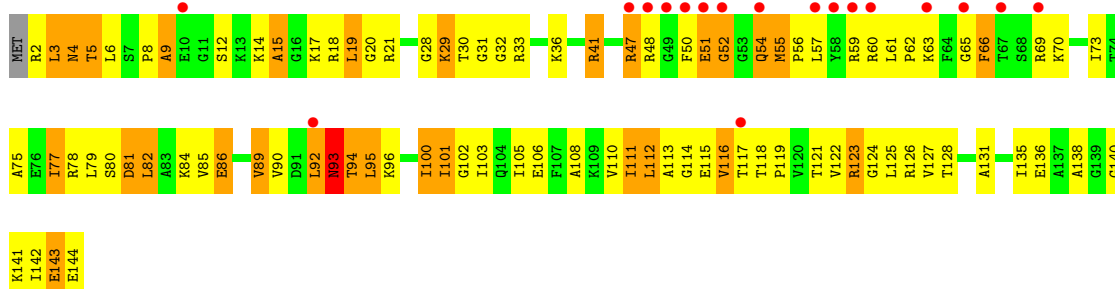
• Molecule 15: 50S ribosomal protein L34

Chain 2:



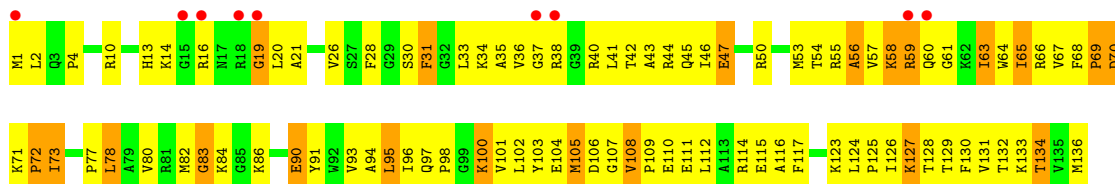
• Molecule 16: 50S ribosomal protein L15

Chain L:



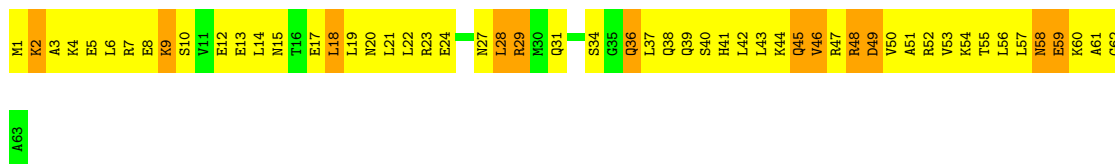
• Molecule 17: 50S ribosomal protein L16

Chain M:



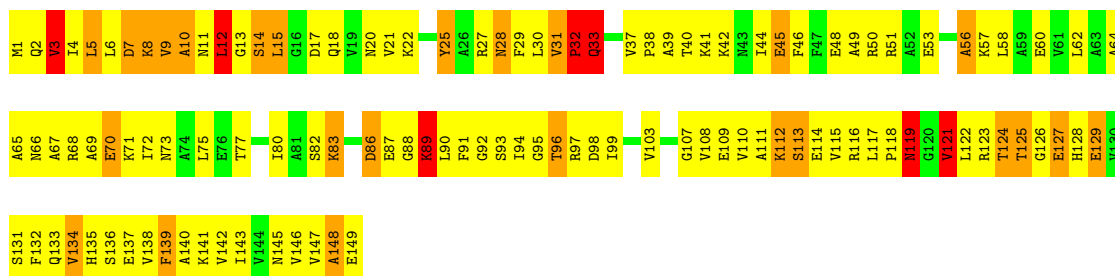
• Molecule 18: 50S ribosomal protein L29

Chain X:



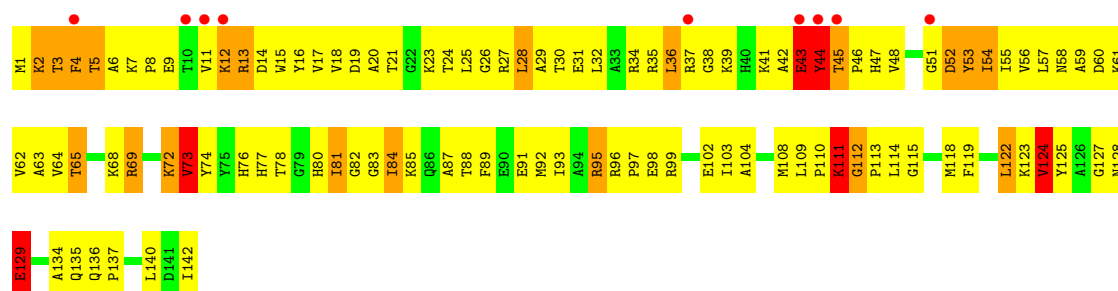
• Molecule 19: 50S ribosomal protein L9

Chain H:



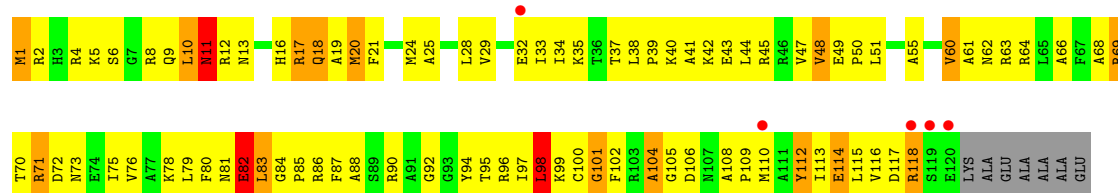
• Molecule 20: 50S ribosomal protein L13

Chain J:



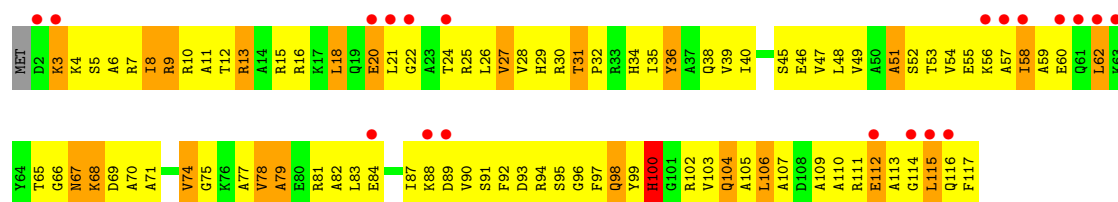
- Molecule 21: 50S ribosomal protein L17

Chain N:



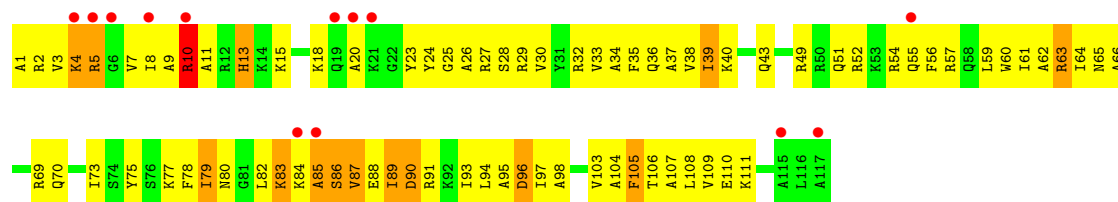
- Molecule 22: 50S ribosomal protein L18

Chain O:



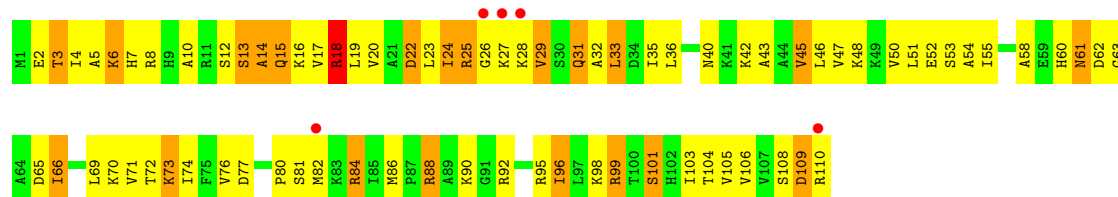
- Molecule 23: 50S ribosomal protein L20

Chain Q:



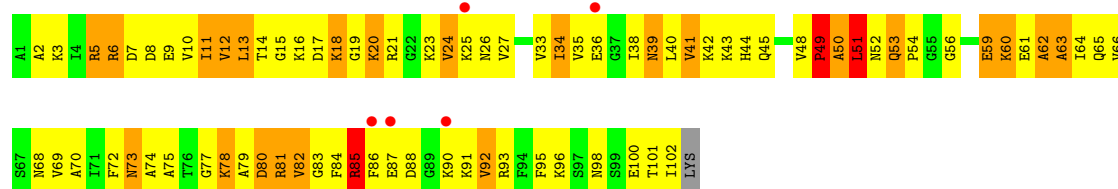
- Molecule 24: 50S ribosomal protein L22

Chain S:



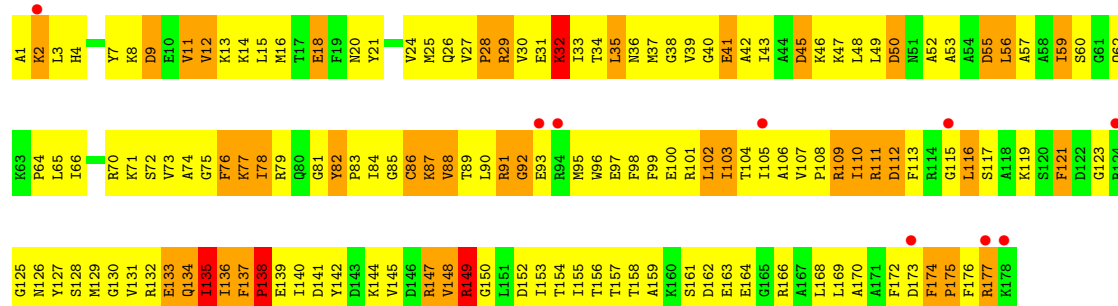
- Molecule 25: 50S ribosomal protein L24

Chain U: 



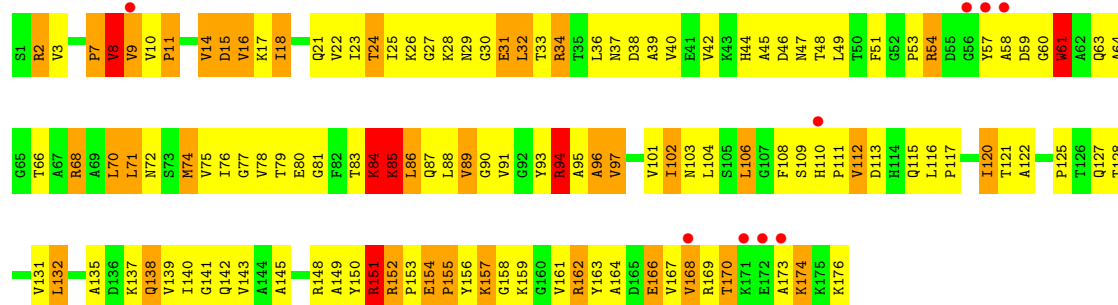
- Molecule 26: 50S ribosomal protein L5

Chain F: 



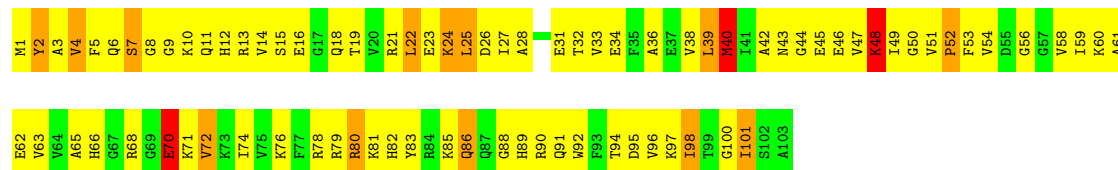
- Molecule 27: 50S ribosomal protein L6

Chain G: 



- Molecule 28: 50S ribosomal protein L21

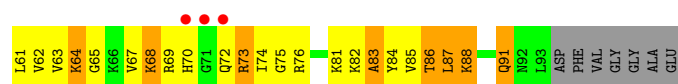
Chain R: 



- Molecule 29: 50S ribosomal protein L23

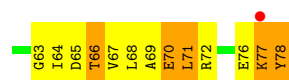
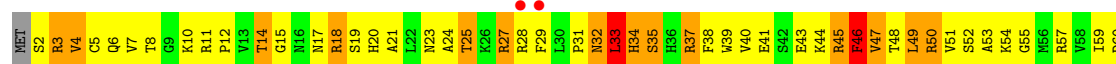
Chain T: 





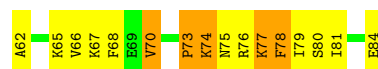
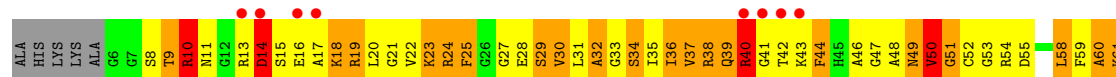
• Molecule 30: 50S ribosomal protein L28

Chain Z:



• Molecule 31: 50S ribosomal protein L27

Chain W:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 70.00 – 3.54 138.41 – 3.55 | Depositor EDS |
| % Data completeness (in resolution range) | 88.8 (70.00-3.54) 89.9 (138.41-3.55) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.69 (at 3.58Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.281 , 0.320 0.474 , 0.482 | Depositor DCC |
| R_{free} test set | 30187 reflections (4.81%) | DCC |
| Wilson B-factor (Å ²) | 125.1 | Xtriage |
| Anisotropy | 0.234 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 4.1 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 1 of 627888 reflections (0.000%) | Xtriage |
| F_o, F_c correlation | 0.69 | EDS |
| Total number of atoms | 90294 | wwPDB-VP |
| Average B, all atoms (Å ²) | 55.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.23 | 0/2803 | 0.74 | 0/4371 |
| 2 | B | 0.28 | 9/68314 (0.0%) | 0.78 | 58/106569 (0.1%) |
| 3 | I | 0.25 | 0/1046 | 0.48 | 0/1410 |
| 4 | C | 0.22 | 0/2121 | 0.48 | 0/2852 |
| 5 | D | 0.24 | 0/1586 | 0.48 | 0/2134 |
| 6 | K | 0.24 | 0/939 | 0.53 | 0/1258 |
| 7 | P | 0.24 | 0/929 | 0.50 | 0/1242 |
| 8 | E | 0.24 | 0/1571 | 0.50 | 0/2113 |
| 9 | Y | 0.23 | 0/453 | 0.48 | 0/605 |
| 10 | O | 0.22 | 0/450 | 0.53 | 0/599 |
| 11 | 4 | 0.23 | 0/303 | 0.46 | 0/397 |
| 12 | 1 | 0.27 | 0/416 | 0.48 | 0/554 |
| 13 | 3 | 0.24 | 0/513 | 0.47 | 0/676 |
| 14 | V | 0.25 | 0/766 | 0.42 | 0/1025 |
| 15 | 2 | 0.25 | 0/380 | 0.45 | 0/498 |
| 16 | L | 0.24 | 0/1054 | 0.47 | 0/1403 |
| 17 | M | 0.25 | 0/1093 | 0.47 | 0/1460 |
| 18 | X | 0.24 | 0/510 | 0.52 | 0/677 |
| 19 | H | 0.25 | 0/1122 | 0.47 | 0/1515 |
| 20 | J | 0.23 | 0/1152 | 0.48 | 0/1551 |
| 21 | N | 0.24 | 0/973 | 0.51 | 0/1301 |
| 22 | O | 0.23 | 0/902 | 0.48 | 0/1209 |
| 23 | Q | 0.25 | 0/960 | 0.47 | 0/1278 |
| 24 | S | 0.22 | 0/864 | 0.51 | 0/1156 |
| 25 | U | 0.26 | 0/787 | 0.46 | 0/1051 |
| 26 | F | 0.26 | 0/1444 | 0.50 | 0/1937 |
| 27 | G | 0.23 | 0/1343 | 0.47 | 0/1816 |
| 28 | R | 0.25 | 0/829 | 0.48 | 0/1107 |
| 29 | T | 0.22 | 0/744 | 0.54 | 0/994 |
| 30 | Z | 0.25 | 0/635 | 0.50 | 0/848 |
| 31 | W | 0.28 | 0/603 | 0.48 | 0/797 |
| All | All | 0.27 | 9/97605 (0.0%) | 0.72 | 58/146403 (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 |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 40 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 2 | B | 1086 | A | C5-C6 | -16.38 | 1.26 | 1.41 |
| 2 | B | 1088 | A | C6-N1 | -10.61 | 1.28 | 1.35 |
| 2 | B | 1060 | U | C2-N3 | 8.04 | 1.43 | 1.37 |
| 2 | B | 2276 | G | O3'-P | -8.01 | 1.51 | 1.61 |
| 2 | B | 2280 | G | O3'-P | 7.60 | 1.70 | 1.61 |
| 2 | B | 1086 | A | N7-C5 | -6.66 | 1.35 | 1.39 |
| 2 | B | 1086 | A | N3-C4 | -6.23 | 1.31 | 1.34 |
| 2 | B | 2323 | G | O3'-P | 6.15 | 1.68 | 1.61 |
| 2 | B | 2267 | A | C5-C6 | -5.05 | 1.36 | 1.41 |

All (58) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2 | B | 2204 | G | O5'-P-OP1 | -29.68 | 75.08 | 110.70 |
| 2 | B | 2791 | G | O5'-P-OP2 | -27.65 | 77.52 | 110.70 |
| 2 | B | 2791 | G | O5'-P-OP1 | 17.94 | 132.23 | 110.70 |
| 2 | B | 2204 | G | O5'-P-OP2 | 17.92 | 132.20 | 110.70 |
| 2 | B | 2790 | U | OP2-P-O3' | 14.55 | 137.22 | 105.20 |
| 2 | B | 2203 | U | OP1-P-O3' | 14.49 | 137.07 | 105.20 |
| 2 | B | 1552 | A | N9-C1'-C2' | -9.01 | 102.09 | 112.00 |
| 2 | B | 2272 | U | C5-C4-O4 | -8.46 | 120.83 | 125.90 |
| 2 | B | 773 | U | C5'-C4'-C3' | -8.41 | 102.54 | 116.00 |
| 2 | B | 1088 | A | N1-C6-N6 | -8.30 | 113.62 | 118.60 |
| 2 | B | 1350 | C | C5'-C4'-C3' | -7.43 | 104.11 | 116.00 |
| 2 | B | 1060 | U | C5-C4-O4 | -7.34 | 121.50 | 125.90 |
| 2 | B | 745 | G | C5'-C4'-C3' | -7.30 | 104.32 | 116.00 |
| 2 | B | 1439 | A | N9-C1'-C2' | -7.12 | 104.16 | 112.00 |
| 2 | B | 2733 | A | N9-C1'-C2' | -6.97 | 104.33 | 112.00 |
| 2 | B | 126 | A | C5'-C4'-C3' | 6.96 | 127.14 | 116.00 |
| 2 | B | 1086 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 2 | B | 690 | G | C5'-C4'-C3' | -6.75 | 105.20 | 116.00 |
| 2 | B | 955 | U | C5'-C4'-C3' | -6.61 | 105.43 | 116.00 |
| 2 | B | 1088 | A | C5-C6-N6 | 6.41 | 128.82 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | B | 2199 | A | C5'-C4'-C3' | -6.35 | 105.84 | 116.00 |
| 2 | B | 560 | C | C5'-C4'-C3' | -6.31 | 105.91 | 116.00 |
| 2 | B | 1086 | A | C6-C5-N7 | -6.25 | 127.93 | 132.30 |
| 2 | B | 1126 | A | C5'-C4'-O4' | 6.21 | 116.55 | 109.10 |
| 2 | B | 2096 | C | C5'-C4'-C3' | -6.08 | 106.27 | 116.00 |
| 2 | B | 1397 | U | C5'-C4'-C3' | -6.00 | 106.41 | 116.00 |
| 2 | B | 2790 | U | O3'-P-O5' | -5.94 | 92.72 | 104.00 |
| 2 | B | 2471 | A | C5'-C4'-C3' | -5.90 | 106.56 | 116.00 |
| 2 | B | 2203 | U | O3'-P-O5' | -5.88 | 92.83 | 104.00 |
| 2 | B | 2267 | A | C4-N9-C1' | 5.74 | 136.63 | 126.30 |
| 2 | B | 2619 | C | C5'-C4'-C3' | -5.71 | 106.87 | 116.00 |
| 2 | B | 2894 | G | N9-C1'-C2' | -5.67 | 105.76 | 112.00 |
| 2 | B | 2267 | A | C8-N9-C1' | -5.66 | 117.51 | 127.70 |
| 2 | B | 1567 | G | C5'-C4'-C3' | -5.64 | 106.97 | 116.00 |
| 2 | B | 1060 | U | N1-C2-O2 | -5.62 | 118.86 | 122.80 |
| 2 | B | 2894 | G | C5'-C4'-C3' | -5.57 | 107.08 | 116.00 |
| 2 | B | 2267 | A | C5-C6-N6 | -5.55 | 119.26 | 123.70 |
| 2 | B | 2267 | A | O4'-C1'-N9 | -5.54 | 103.77 | 108.20 |
| 2 | B | 401 | A | C5'-C4'-C3' | 5.54 | 124.86 | 116.00 |
| 2 | B | 1869 | G | N9-C1'-C2' | -5.51 | 105.94 | 112.00 |
| 2 | B | 1086 | A | C2-N3-C4 | -5.47 | 107.87 | 110.60 |
| 2 | B | 1324 | G | C5'-C4'-C3' | -5.47 | 107.25 | 116.00 |
| 2 | B | 973 | A | C5'-C4'-C3' | -5.45 | 107.28 | 116.00 |
| 2 | B | 1634 | A | C5'-C4'-C3' | -5.41 | 107.34 | 116.00 |
| 2 | B | 1060 | U | N3-C2-O2 | 5.32 | 125.92 | 122.20 |
| 2 | B | 1318 | U | C5'-C4'-C3' | -5.32 | 107.50 | 116.00 |
| 2 | B | 1663 | G | C5'-C4'-C3' | -5.27 | 107.57 | 116.00 |
| 2 | B | 1911 | U | C4'-C3'-O3' | 5.25 | 123.50 | 113.00 |
| 2 | B | 1600 | C | C5'-C4'-C3' | -5.24 | 107.61 | 116.00 |
| 2 | B | 1818 | U | C4'-C3'-O3' | -5.21 | 98.47 | 109.40 |
| 2 | B | 785 | G | C5'-C4'-C3' | -5.20 | 107.67 | 116.00 |
| 2 | B | 2283 | C | P-O5'-C5' | 5.16 | 129.15 | 120.90 |
| 2 | B | 2272 | U | N1-C1'-C2' | -5.16 | 106.33 | 112.00 |
| 2 | B | 479 | A | C4'-C3'-O3' | -5.15 | 98.58 | 109.40 |
| 2 | B | 2285 | C | C5'-C4'-C3' | -5.14 | 107.77 | 116.00 |
| 2 | B | 700 | G | C5'-C4'-C3' | -5.09 | 107.85 | 116.00 |
| 2 | B | 386 | G | C5'-C4'-C3' | -5.04 | 107.93 | 116.00 |
| 2 | B | 1552 | A | C4'-C3'-O3' | 5.02 | 123.03 | 113.00 |

There are no chirality outliers.

All (40) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 2 | B | 1047 | G | Sidechain |
| 2 | B | 1060 | U | Sidechain |
| 2 | B | 1086 | A | Sidechain |
| 2 | B | 1088 | A | Sidechain |
| 2 | B | 1377 | G | Sidechain |
| 2 | B | 1432 | G | Sidechain |
| 2 | B | 1439 | A | Sidechain |
| 2 | B | 1533 | C | Sidechain |
| 2 | B | 1546 | G | Sidechain |
| 2 | B | 1572 | A | Sidechain |
| 2 | B | 1734 | G | Sidechain |
| 2 | B | 1814 | G | Sidechain |
| 2 | B | 1828 | G | Sidechain |
| 2 | B | 1869 | G | Sidechain |
| 2 | B | 2062 | A | Sidechain |
| 2 | B | 221 | A | Sidechain |
| 2 | B | 222 | A | Sidechain |
| 2 | B | 2267 | A | Sidechain |
| 2 | B | 2272 | U | Sidechain |
| 2 | B | 2279 | G | Sidechain |
| 2 | B | 232 | G | Sidechain |
| 2 | B | 2454 | G | Sidechain |
| 2 | B | 2471 | A | Sidechain |
| 2 | B | 2503 | A | Sidechain |
| 2 | B | 2638 | G | Sidechain |
| 2 | B | 2733 | A | Sidechain |
| 2 | B | 2770 | G | Sidechain |
| 2 | B | 2834 | G | Sidechain |
| 2 | B | 2848 | G | Sidechain |
| 2 | B | 2857 | G | Sidechain |
| 2 | B | 2868 | A | Sidechain |
| 2 | B | 2883 | A | Sidechain |
| 2 | B | 299 | A | Sidechain |
| 2 | B | 500 | G | Sidechain |
| 2 | B | 51 | G | Sidechain |
| 2 | B | 630 | G | Sidechain |
| 2 | B | 633 | A | Sidechain |
| 2 | B | 727 | A | Sidechain |
| 2 | B | 729 | G | Sidechain |
| 2 | B | 757 | G | Sidechain |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2507 | 0 | 1270 | 96 | 0 |
| 2 | B | 60995 | 0 | 30677 | 2298 | 0 |
| 3 | I | 1032 | 0 | 1088 | 176 | 0 |
| 4 | C | 2082 | 0 | 2157 | 245 | 0 |
| 5 | D | 1565 | 0 | 1616 | 186 | 0 |
| 6 | K | 930 | 0 | 1000 | 108 | 0 |
| 7 | P | 917 | 0 | 965 | 107 | 0 |
| 8 | E | 1552 | 0 | 1619 | 153 | 0 |
| 9 | Y | 449 | 0 | 491 | 59 | 0 |
| 10 | 0 | 444 | 0 | 461 | 45 | 0 |
| 11 | 4 | 302 | 0 | 340 | 42 | 0 |
| 12 | 1 | 409 | 0 | 440 | 47 | 0 |
| 13 | 3 | 504 | 0 | 574 | 45 | 0 |
| 14 | V | 753 | 0 | 780 | 97 | 0 |
| 15 | 2 | 377 | 0 | 418 | 34 | 0 |
| 16 | L | 1045 | 0 | 1117 | 153 | 0 |
| 17 | M | 1074 | 0 | 1157 | 119 | 0 |
| 18 | X | 509 | 0 | 543 | 72 | 0 |
| 19 | H | 1111 | 0 | 1148 | 150 | 0 |
| 20 | J | 1129 | 0 | 1162 | 144 | 0 |
| 21 | N | 960 | 0 | 1000 | 118 | 0 |
| 22 | O | 892 | 0 | 923 | 103 | 0 |
| 23 | Q | 947 | 0 | 1022 | 141 | 0 |
| 24 | S | 857 | 0 | 922 | 87 | 0 |
| 25 | U | 779 | 0 | 834 | 114 | 0 |
| 26 | F | 1420 | 0 | 1460 | 224 | 0 |
| 27 | G | 1323 | 0 | 1374 | 191 | 0 |
| 28 | R | 816 | 0 | 839 | 112 | 0 |
| 29 | T | 738 | 0 | 807 | 128 | 0 |
| 30 | Z | 625 | 0 | 652 | 77 | 0 |
| 31 | W | 596 | 0 | 610 | 131 | 0 |
| 32 | B | 111 | 0 | 0 | 0 | 0 |
| 33 | 4 | 1 | 0 | 0 | 0 | 0 |
| 34 | B | 31 | 0 | 39 | 0 | 0 |
| 35 | B | 502 | 0 | 0 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35 | C | 4 | 0 | 0 | 0 | 0 |
| 35 | E | 2 | 0 | 0 | 0 | 0 |
| 35 | L | 4 | 0 | 0 | 0 | 0 |
| All | All | 90294 | 0 | 59505 | 5289 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

All (5289) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:1099:G:H8 | 3:I:3:LYS:N | 1.42 | 1.17 |
| 2:B:855:G:H21 | 31:W:23:LYS:HG2 | 1.12 | 1.14 |
| 5:D:106:LYS:HB3 | 5:D:206:ALA:H | 1.13 | 1.09 |
| 2:B:1098:A:H3' | 3:I:3:LYS:CA | 1.84 | 1.07 |
| 16:L:143:GLU:HG2 | 16:L:144:GLU:H | 1.17 | 1.07 |
| 4:C:144:GLU:HA | 4:C:151:GLY:HA2 | 1.39 | 1.05 |
| 25:U:85:ARG:HD3 | 25:U:86:PHE:H | 1.20 | 1.04 |
| 2:B:1099:G:O5' | 3:I:4:VAL:N | 1.89 | 1.04 |
| 2:B:1099:G:C8 | 3:I:3:LYS:N | 2.27 | 1.03 |
| 2:B:1098:A:H3' | 3:I:3:LYS:HA | 1.35 | 1.02 |
| 21:N:37:THR:HG22 | 21:N:39:PRO:HD2 | 1.38 | 1.02 |
| 8:E:5:LEU:HD12 | 8:E:10:SER:HB2 | 1.41 | 1.02 |
| 18:X:28:LEU:HD13 | 18:X:37:LEU:HD11 | 1.41 | 1.02 |
| 2:B:45:G:H5'' | 2:B:46:G:H5' | 1.42 | 1.01 |
| 2:B:1024:G:H3' | 2:B:1025:G:H5'' | 1.43 | 1.00 |
| 28:R:60:LYS:H | 28:R:100:GLY:HA3 | 1.25 | 0.99 |
| 27:G:15:ASP:HB3 | 27:G:26:LYS:H | 1.26 | 0.99 |
| 8:E:155:GLU:HA | 8:E:158:PHE:HB3 | 1.44 | 0.98 |
| 27:G:8:VAL:HG11 | 27:G:49:LEU:H | 1.26 | 0.98 |
| 2:B:2579:C:H1' | 5:D:130:GLN:HE22 | 1.23 | 0.98 |
| 2:B:1993:U:H4' | 5:D:133:THR:HG21 | 1.43 | 0.97 |
| 6:K:35:VAL:HG23 | 6:K:36:GLY:H | 1.28 | 0.97 |
| 23:Q:63:ARG:HH22 | 23:Q:96:ASP:HA | 1.27 | 0.97 |
| 19:H:62:LEU:HG | 19:H:66:ASN:HD21 | 1.29 | 0.97 |
| 7:P:63:ILE:HA | 7:P:68:GLY:HA2 | 1.47 | 0.97 |
| 2:B:1812:U:H1' | 4:C:43:ASN:HD21 | 1.28 | 0.97 |
| 19:H:2:GLN:HA | 19:H:20:ASN:HA | 1.46 | 0.97 |
| 5:D:29:VAL:HB | 5:D:98:VAL:HG22 | 1.44 | 0.96 |
| 5:D:10:GLY:HA3 | 5:D:26:VAL:H | 1.26 | 0.96 |
| 31:W:49:ASN:HB2 | 31:W:60:ALA:HA | 1.45 | 0.96 |
| 2:B:2379:G:H4' | 22:O:21:LEU:HD11 | 1.44 | 0.96 |
| 19:H:86:ASP:HB2 | 19:H:89:LYS:HD3 | 1.48 | 0.95 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 19:H:31:VAL:HB | 19:H:32:PRO:CD | 1.96 | 0.95 |
| 4:C:129:LEU:HD23 | 4:C:130:PRO:HD2 | 1.49 | 0.95 |
| 19:H:90:LEU:HB2 | 19:H:123:ARG:HA | 1.48 | 0.95 |
| 5:D:5:VAL:H | 5:D:32:ASN:ND2 | 1.65 | 0.95 |
| 29:T:67:VAL:HB | 29:T:76:ARG:HG3 | 1.47 | 0.93 |
| 2:B:1099:G:H8 | 3:I:3:LYS:H | 1.10 | 0.93 |
| 7:P:13:LYS:HD2 | 7:P:76:HIS:HA | 1.48 | 0.93 |
| 14:V:42:LEU:HD12 | 14:V:47:VAL:HG21 | 1.50 | 0.92 |
| 23:Q:4:LYS:HE2 | 23:Q:7:VAL:HG22 | 1.52 | 0.92 |
| 2:B:858:G:N3 | 2:B:2268:A:H2' | 1.84 | 0.92 |
| 4:C:183:VAL:HG13 | 4:C:185:ALA:H | 1.35 | 0.92 |
| 23:Q:111:LYS:HB2 | 28:R:48:LYS:HZ2 | 1.32 | 0.91 |
| 2:B:2266:A:H4' | 2:B:2267:A:N7 | 1.85 | 0.91 |
| 2:B:27:G:H22 | 2:B:512:G:H2' | 1.34 | 0.91 |
| 17:M:19:GLY:H | 17:M:38:ARG:HH12 | 1.16 | 0.91 |
| 6:K:71:ARG:HA | 6:K:71:ARG:HE | 1.33 | 0.91 |
| 2:B:2366:A:H4' | 31:W:61:LYS:HE2 | 1.53 | 0.91 |
| 2:B:79:C:HO2' | 2:B:346:A:H8 | 1.19 | 0.91 |
| 2:B:704:G:H2' | 2:B:726:G:H22 | 1.35 | 0.90 |
| 29:T:11:LEU:HD22 | 29:T:11:LEU:H | 1.36 | 0.90 |
| 2:B:1175:A:H3' | 2:B:1176:U:H5' | 1.53 | 0.90 |
| 1:A:98:G:H1 | 14:V:14:LYS:HB2 | 1.36 | 0.90 |
| 7:P:4:ILE:HG22 | 7:P:5:LYS:H | 1.34 | 0.90 |
| 26:F:71:LYS:HE2 | 26:F:73:VAL:HB | 1.53 | 0.90 |
| 2:B:2306:C:H3' | 2:B:2307:G:H5' | 1.53 | 0.89 |
| 4:C:64:VAL:O | 4:C:65:ASP:HB3 | 1.72 | 0.89 |
| 11:4:7:VAL:HG13 | 11:4:8:LYS:H | 1.37 | 0.89 |
| 5:D:106:LYS:HB3 | 5:D:206:ALA:N | 1.85 | 0.89 |
| 29:T:69:ARG:HB3 | 29:T:74:ILE:HA | 1.53 | 0.89 |
| 2:B:1060:U:N3 | 2:B:1088:A:N7 | 2.21 | 0.89 |
| 27:G:84:LYS:HG2 | 27:G:85:LYS:H | 1.37 | 0.89 |
| 2:B:1244:A:H5'' | 16:L:8:PRO:HD3 | 1.54 | 0.89 |
| 18:X:37:LEU:HD23 | 18:X:39:GLN:H | 1.37 | 0.89 |
| 21:N:83:LEU:HA | 21:N:86:ARG:HG3 | 1.53 | 0.89 |
| 5:D:5:VAL:H | 5:D:32:ASN:HD21 | 0.93 | 0.88 |
| 18:X:12:GLU:HA | 18:X:15:ASN:HD21 | 1.38 | 0.88 |
| 24:S:26:GLY:H | 24:S:71:VAL:HG13 | 1.35 | 0.88 |
| 2:B:281:C:H2' | 2:B:282:A:C8 | 2.08 | 0.88 |
| 2:B:2502:G:H5' | 2:B:2503:A:H5'' | 1.55 | 0.88 |
| 2:B:495:G:H21 | 24:S:61:ASN:HD21 | 1.14 | 0.88 |
| 28:R:8:GLY:HA3 | 28:R:23:GLU:HB2 | 1.56 | 0.88 |
| 27:G:8:VAL:HG21 | 27:G:49:LEU:HB2 | 1.56 | 0.88 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 29:T:29:THR:HA | 29:T:86:THR:HA | 1.55 | 0.88 |
| 17:M:2:LEU:HD23 | 17:M:46:ILE:HD11 | 1.56 | 0.88 |
| 24:S:24:ILE:HG22 | 24:S:71:VAL:HG11 | 1.56 | 0.88 |
| 26:F:135:ILE:HD11 | 26:F:137:PHE:HB3 | 1.52 | 0.88 |
| 7:P:26:GLU:HG3 | 7:P:43:GLU:HG2 | 1.55 | 0.88 |
| 4:C:180:MET:HB3 | 4:C:267:VAL:HG23 | 1.56 | 0.87 |
| 24:S:73:LYS:HE3 | 24:S:74:ILE:H | 1.39 | 0.87 |
| 2:B:1099:G:H5'' | 3:I:3:LYS:N | 1.90 | 0.87 |
| 2:B:547:A:H5' | 2:B:548:G:H21 | 1.40 | 0.87 |
| 19:H:46:PHE:HA | 19:H:50:ARG:HH21 | 1.37 | 0.87 |
| 31:W:39:GLN:HE21 | 31:W:42:THR:HB | 1.39 | 0.87 |
| 31:W:17:ALA:HA | 31:W:35:ILE:HG23 | 1.54 | 0.87 |
| 2:B:2886:A:H62 | 10:O:39:ARG:NE | 1.72 | 0.87 |
| 20:J:58:ASN:HA | 20:J:127:GLY:HA2 | 1.57 | 0.87 |
| 2:B:1099:G:P | 3:I:3:LYS:HA | 2.15 | 0.87 |
| 6:K:47:ILE:HG12 | 6:K:48:PRO:HD2 | 1.53 | 0.87 |
| 16:L:82:LEU:HD23 | 16:L:90:VAL:HG21 | 1.57 | 0.86 |
| 28:R:2:TYR:HB2 | 28:R:42:ALA:HB2 | 1.57 | 0.86 |
| 2:B:742:A:H2' | 2:B:743:A:H8 | 1.40 | 0.86 |
| 16:L:123:ARG:HA | 16:L:143:GLU:HB3 | 1.57 | 0.86 |
| 2:B:2653:U:H3' | 2:B:2654:A:H2' | 1.58 | 0.86 |
| 2:B:1287:A:OP1 | 21:N:104:ALA:HB3 | 1.76 | 0.86 |
| 27:G:34:ARG:HH11 | 27:G:34:ARG:H | 1.21 | 0.86 |
| 23:Q:105:PHE:HA | 23:Q:108:LEU:HD12 | 1.58 | 0.85 |
| 21:N:38:LEU:HB3 | 21:N:39:PRO:HD3 | 1.57 | 0.85 |
| 28:R:7:SER:HB2 | 28:R:22:LEU:HB3 | 1.59 | 0.85 |
| 30:Z:38:PHE:HE2 | 30:Z:51:VAL:HG21 | 1.41 | 0.85 |
| 16:L:29:LYS:HG3 | 16:L:30:THR:HG23 | 1.58 | 0.85 |
| 17:M:19:GLY:HA2 | 17:M:97:GLN:HB2 | 1.58 | 0.85 |
| 29:T:15:HIS:H | 29:T:32:LEU:HA | 1.40 | 0.85 |
| 19:H:5:LEU:HD12 | 19:H:17:ASP:HB2 | 1.59 | 0.85 |
| 21:N:101:GLY:HA2 | 21:N:110:MET:N | 1.91 | 0.85 |
| 2:B:1168:G:H2' | 2:B:1169:A:C8 | 2.12 | 0.85 |
| 7:P:75:THR:HG23 | 7:P:76:HIS:H | 1.42 | 0.84 |
| 2:B:1911:U:H2' | 2:B:1918:A:N1 | 1.92 | 0.84 |
| 2:B:2720:U:H5'' | 7:P:52:ARG:NH2 | 1.92 | 0.84 |
| 2:B:855:G:N2 | 31:W:23:LYS:HG2 | 1.91 | 0.84 |
| 5:D:5:VAL:N | 5:D:32:ASN:HD21 | 1.75 | 0.84 |
| 21:N:2:ARG:HG2 | 21:N:5:LYS:HB2 | 1.59 | 0.84 |
| 31:W:50:VAL:HG23 | 31:W:61:LYS:HD3 | 1.60 | 0.84 |
| 2:B:558:U:OP1 | 20:J:113:PRO:HG2 | 1.77 | 0.84 |
| 2:B:2179:C:H2' | 2:B:2179:C:O2 | 1.78 | 0.84 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:2529:G:H4' | 27:G:174:LYS:HG3 | 1.58 | 0.84 |
| 23:Q:65:ASN:HD21 | 23:Q:69:ARG:HH11 | 1.22 | 0.84 |
| 20:J:29:ALA:HA | 20:J:32:LEU:HD12 | 1.60 | 0.84 |
| 14:V:14:LYS:HE2 | 14:V:18:ARG:HH21 | 1.41 | 0.84 |
| 2:B:90:U:H3' | 2:B:91:A:H5'' | 1.59 | 0.84 |
| 3:I:27:LEU:H | 3:I:27:LEU:HD23 | 1.43 | 0.83 |
| 26:F:11:VAL:HG12 | 26:F:12:VAL:H | 1.41 | 0.83 |
| 2:B:1019:U:H2' | 2:B:1020:A:C8 | 2.14 | 0.83 |
| 2:B:1437:C:H2' | 2:B:1438:U:C6 | 2.13 | 0.83 |
| 5:D:91:THR:HG23 | 5:D:92:VAL:H | 1.43 | 0.83 |
| 5:D:148:GLN:HB2 | 5:D:152:PRO:HG2 | 1.58 | 0.83 |
| 21:N:2:ARG:HA | 21:N:5:LYS:HD3 | 1.58 | 0.83 |
| 26:F:168:LEU:HD13 | 26:F:169:LEU:H | 1.44 | 0.83 |
| 30:Z:54:LYS:HA | 30:Z:57:ARG:HD3 | 1.60 | 0.83 |
| 2:B:675:A:H4' | 8:E:62:GLN:HE22 | 1.44 | 0.83 |
| 20:J:81:ILE:HG23 | 20:J:82:GLY:H | 1.44 | 0.83 |
| 2:B:161:A:H3' | 2:B:162:U:H5'' | 1.61 | 0.83 |
| 2:B:1099:G:P | 3:I:4:VAL:H | 2.01 | 0.83 |
| 15:2:21:ARG:HD3 | 15:2:43:THR:HG21 | 1.61 | 0.83 |
| 2:B:856:G:H1' | 31:W:23:LYS:HB3 | 1.61 | 0.83 |
| 2:B:404:A:H4' | 2:B:405:U:H5' | 1.61 | 0.83 |
| 29:T:57:VAL:HG22 | 29:T:58:VAL:H | 1.43 | 0.82 |
| 2:B:2073:C:H5'' | 4:C:227:VAL:HG12 | 1.59 | 0.82 |
| 24:S:24:ILE:HD11 | 24:S:36:LEU:HD11 | 1.61 | 0.82 |
| 2:B:126:A:H5' | 15:2:19:ARG:HG3 | 1.60 | 0.82 |
| 3:I:121:ILE:HD13 | 3:I:121:ILE:H | 1.44 | 0.82 |
| 8:E:145:ASP:HA | 8:E:166:LYS:HB3 | 1.61 | 0.82 |
| 23:Q:63:ARG:NH2 | 23:Q:96:ASP:HA | 1.93 | 0.82 |
| 30:Z:7:VAL:HG13 | 30:Z:8:THR:HG23 | 1.59 | 0.82 |
| 2:B:28:A:H61 | 2:B:512:G:H1' | 1.43 | 0.82 |
| 2:B:1060:U:C2 | 2:B:1088:A:N7 | 2.48 | 0.82 |
| 2:B:142:A:H2' | 2:B:143:C:C6 | 2.15 | 0.82 |
| 24:S:76:VAL:HG12 | 24:S:103:ILE:HA | 1.62 | 0.82 |
| 30:Z:35:SER:HB3 | 30:Z:50:ARG:HG3 | 1.58 | 0.82 |
| 11:4:17:VAL:HG12 | 11:4:18:LYS:H | 1.44 | 0.82 |
| 2:B:1283:G:H22 | 2:B:1286:A:H5' | 1.45 | 0.82 |
| 9:Y:12:ALA:HA | 9:Y:15:ARG:HD3 | 1.60 | 0.81 |
| 6:K:41:ILE:HG13 | 6:K:42:THR:N | 1.93 | 0.81 |
| 22:O:15:ARG:HH21 | 22:O:95:SER:HB3 | 1.45 | 0.81 |
| 2:B:1099:G:H8 | 3:I:3:LYS:CA | 1.93 | 0.81 |
| 5:D:24:VAL:HG21 | 5:D:188:LEU:HB3 | 1.61 | 0.81 |
| 17:M:134:THR:HG22 | 17:M:136:MET:H | 1.45 | 0.81 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 29:T:11:LEU:HA | 29:T:34:VAL:HG12 | 1.62 | 0.81 |
| 2:B:495:G:N2 | 24:S:61:ASN:HD21 | 1.77 | 0.81 |
| 17:M:71:LYS:HE3 | 17:M:73:ILE:HD11 | 1.62 | 0.81 |
| 26:F:62:GLN:HG3 | 26:F:91:ARG:HH11 | 1.43 | 0.81 |
| 31:W:37:VAL:HG12 | 31:W:38:ARG:H | 1.43 | 0.81 |
| 30:Z:64:ILE:HD12 | 30:Z:64:ILE:H | 1.43 | 0.81 |
| 16:L:6:LEU:HD23 | 16:L:6:LEU:H | 1.45 | 0.81 |
| 24:S:4:ILE:HG22 | 24:S:106:VAL:HG13 | 1.62 | 0.81 |
| 30:Z:33:LEU:HA | 30:Z:52:SER:HA | 1.61 | 0.81 |
| 2:B:359:G:H2' | 2:B:360:U:H5' | 1.62 | 0.81 |
| 1:A:32:U:H4' | 1:A:52:A:H62 | 1.44 | 0.81 |
| 26:F:128:SER:HB3 | 26:F:154:THR:HG23 | 1.60 | 0.81 |
| 20:J:17:VAL:HG23 | 20:J:137:PRO:HB2 | 1.62 | 0.81 |
| 25:U:85:ARG:HD3 | 25:U:86:PHE:N | 1.95 | 0.81 |
| 2:B:1338:G:H4' | 29:T:18:GLU:HG3 | 1.63 | 0.81 |
| 19:H:31:VAL:HB | 19:H:32:PRO:HD2 | 1.60 | 0.81 |
| 21:N:102:PHE:H | 21:N:109:PRO:HA | 1.46 | 0.81 |
| 19:H:62:LEU:HG | 19:H:66:ASN:ND2 | 1.95 | 0.80 |
| 3:I:11:GLN:HG2 | 3:I:55:PRO:HB3 | 1.63 | 0.80 |
| 22:O:5:SER:HA | 22:O:8:ILE:HD12 | 1.62 | 0.80 |
| 2:B:1141:U:H4' | 2:B:1142:A:O4' | 1.80 | 0.80 |
| 2:B:1080:A:H4' | 3:I:126:ARG:HD3 | 1.61 | 0.80 |
| 5:D:184:ARG:HG3 | 5:D:186:LEU:HB2 | 1.63 | 0.80 |
| 3:I:21:PRO:HB2 | 3:I:22:PRO:HD3 | 1.64 | 0.80 |
| 2:B:138:U:O3' | 2:B:139:U:H3' | 1.81 | 0.80 |
| 12:1:49:LYS:HG3 | 12:1:50:GLU:H | 1.46 | 0.80 |
| 2:B:1099:G:OP2 | 3:I:3:LYS:HA | 1.82 | 0.80 |
| 16:L:116:VAL:HG13 | 16:L:117:THR:H | 1.44 | 0.80 |
| 2:B:1099:G:H5'' | 3:I:2:LYS:C | 2.01 | 0.80 |
| 24:S:66:ILE:HD13 | 24:S:66:ILE:H | 1.45 | 0.80 |
| 9:Y:16:LEU:HD22 | 9:Y:16:LEU:H | 1.46 | 0.79 |
| 26:F:30:VAL:HG21 | 26:F:96:TRP:HE1 | 1.48 | 0.79 |
| 23:Q:91:ARG:HH12 | 28:R:10:LYS:HB3 | 1.47 | 0.79 |
| 2:B:742:A:H2' | 2:B:743:A:C8 | 2.16 | 0.79 |
| 9:Y:6:ILE:HG21 | 9:Y:47:ILE:HD12 | 1.63 | 0.79 |
| 25:U:14:THR:HB | 25:U:68:ASN:HB3 | 1.63 | 0.79 |
| 12:1:4:ILE:HB | 12:1:27:ARG:HG3 | 1.65 | 0.79 |
| 2:B:1098:A:H2' | 3:I:4:VAL:N | 1.98 | 0.79 |
| 22:O:49:VAL:HG11 | 22:O:82:ALA:HA | 1.65 | 0.79 |
| 14:V:42:LEU:HD23 | 14:V:42:LEU:H | 1.47 | 0.79 |
| 30:Z:31:PRO:HB2 | 30:Z:33:LEU:HD11 | 1.63 | 0.79 |
| 2:B:1082:U:C4 | 2:B:1086:A:C2 | 2.71 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 31:W:9:THR:HG23 | 31:W:10:ARG:HD3 | 1.63 | 0.79 |
| 2:B:2769:U:H2' | 2:B:2770:G:H8 | 1.47 | 0.79 |
| 16:L:80:SER:HA | 16:L:115:GLU:HB2 | 1.63 | 0.79 |
| 2:B:28:A:N6 | 2:B:512:G:H1' | 1.98 | 0.78 |
| 19:H:135:HIS:HB3 | 19:H:138:VAL:HB | 1.62 | 0.78 |
| 8:E:60:TRP:O | 8:E:61:ARG:HB2 | 1.82 | 0.78 |
| 2:B:2143:C:H3' | 2:B:2144:G:H8 | 1.48 | 0.78 |
| 6:K:54:LYS:H | 6:K:54:LYS:HD2 | 1.49 | 0.78 |
| 24:S:36:LEU:HD22 | 24:S:36:LEU:H | 1.46 | 0.78 |
| 7:P:20:ARG:HG3 | 7:P:21:PRO:HD2 | 1.64 | 0.78 |
| 29:T:29:THR:H | 29:T:91:GLN:HE22 | 1.30 | 0.78 |
| 2:B:2365:G:H4' | 31:W:59:PHE:CD1 | 2.19 | 0.78 |
| 3:I:45:THR:HA | 3:I:48:ILE:HG22 | 1.66 | 0.78 |
| 4:C:76:VAL:HG12 | 4:C:114:GLN:HG2 | 1.65 | 0.78 |
| 25:U:49:PRO:HA | 25:U:53:GLN:HG3 | 1.63 | 0.78 |
| 16:L:143:GLU:HG2 | 16:L:144:GLU:N | 1.97 | 0.78 |
| 25:U:84:PHE:O | 25:U:85:ARG:HB2 | 1.82 | 0.78 |
| 27:G:24:THR:HA | 27:G:34:ARG:HA | 1.64 | 0.78 |
| 17:M:19:GLY:HA2 | 17:M:98:PRO:HD2 | 1.64 | 0.78 |
| 29:T:11:LEU:HD21 | 29:T:46:ALA:HB1 | 1.65 | 0.78 |
| 26:F:126:ASN:HB3 | 26:F:156:THR:HA | 1.63 | 0.78 |
| 19:H:65:ALA:HB1 | 19:H:138:VAL:HG21 | 1.65 | 0.78 |
| 2:B:1324:G:H1' | 2:B:1616:A:N6 | 1.98 | 0.77 |
| 2:B:2148:G:H1' | 2:B:2149:U:C5 | 2.18 | 0.77 |
| 27:G:166:GLU:HG2 | 27:G:168:VAL:HG23 | 1.66 | 0.77 |
| 2:B:27:G:N2 | 2:B:512:G:H2' | 2.00 | 0.77 |
| 30:Z:6:GLN:HE22 | 30:Z:50:ARG:H | 1.33 | 0.77 |
| 2:B:1454:C:H1' | 21:N:60:VAL:HG13 | 1.67 | 0.77 |
| 28:R:72:VAL:HG23 | 28:R:89:HIS:HB3 | 1.66 | 0.77 |
| 30:Z:7:VAL:HG21 | 30:Z:59:ILE:HD11 | 1.66 | 0.77 |
| 4:C:143:VAL:HB | 4:C:153:LEU:HB2 | 1.65 | 0.77 |
| 26:F:163:GLU:HA | 26:F:166:ARG:HD2 | 1.66 | 0.77 |
| 2:B:1447:C:H2' | 2:B:1448:G:H8 | 1.50 | 0.77 |
| 20:J:57:LEU:HG | 20:J:128:ASN:H | 1.49 | 0.77 |
| 29:T:54:GLU:HB3 | 29:T:88:LYS:HB2 | 1.67 | 0.77 |
| 25:U:81:ARG:HH21 | 25:U:81:ARG:H | 1.33 | 0.77 |
| 19:H:125:THR:HA | 19:H:146:VAL:HB | 1.67 | 0.77 |
| 19:H:96:THR:HG23 | 19:H:97:ARG:H | 1.49 | 0.76 |
| 2:B:1913:A:H4' | 2:B:1914:C:H5'' | 1.67 | 0.76 |
| 12:1:6:GLU:HB2 | 12:1:52:LYS:HZ1 | 1.48 | 0.76 |
| 2:B:1178:C:H2' | 2:B:1179:G:H8 | 1.49 | 0.76 |
| 3:I:55:PRO:HD3 | 3:I:74:PRO:HD3 | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 21:N:24:MET:HG2 | 21:N:44:LEU:HD22 | 1.67 | 0.76 |
| 30:Z:5:CYS:HB3 | 30:Z:10:LYS:H | 1.50 | 0.76 |
| 25:U:80:ASP:HB2 | 25:U:96:LYS:N | 2.01 | 0.76 |
| 2:B:1080:A:H2' | 2:B:1081:U:H6 | 1.49 | 0.76 |
| 2:B:1097:U:H2' | 2:B:1098:A:O4' | 1.84 | 0.76 |
| 5:D:105:LYS:HD2 | 5:D:177:VAL:HG22 | 1.68 | 0.76 |
| 3:I:72:THR:HG21 | 3:I:112:LYS:HA | 1.67 | 0.76 |
| 6:K:76:VAL:H | 7:P:72:VAL:HG23 | 1.51 | 0.76 |
| 2:B:2336:A:H61 | 31:W:40:ARG:HG3 | 1.51 | 0.76 |
| 3:I:105:LEU:HD13 | 3:I:129:GLU:HG2 | 1.66 | 0.76 |
| 18:X:3:ALA:HA | 18:X:6:LEU:HD23 | 1.68 | 0.76 |
| 18:X:31:GLN:HG2 | 18:X:37:LEU:HB2 | 1.67 | 0.76 |
| 22:O:27:VAL:HG21 | 22:O:40:ILE:HD12 | 1.68 | 0.76 |
| 2:B:1592:C:H2' | 2:B:1593:A:H8 | 1.51 | 0.76 |
| 9:Y:2:LYS:HD3 | 9:Y:2:LYS:H | 1.51 | 0.76 |
| 25:U:70:ALA:HB1 | 25:U:79:ALA:HB3 | 1.66 | 0.76 |
| 17:M:126:ILE:H | 17:M:126:ILE:HD12 | 1.49 | 0.76 |
| 27:G:30:GLY:HA3 | 27:G:78:VAL:HA | 1.67 | 0.76 |
| 24:S:26:GLY:N | 24:S:71:VAL:HG13 | 2.00 | 0.76 |
| 2:B:1172:C:H2' | 2:B:1173:U:O4' | 1.86 | 0.76 |
| 2:B:1080:A:H4' | 3:I:126:ARG:CD | 2.16 | 0.76 |
| 2:B:2787:C:H1' | 5:D:63:PRO:HG3 | 1.68 | 0.76 |
| 2:B:1080:A:O2' | 3:I:126:ARG:HD2 | 1.86 | 0.75 |
| 14:V:9:ARG:NH2 | 14:V:12:GLN:HA | 2.01 | 0.75 |
| 2:B:2591:C:H2' | 2:B:2592:G:C8 | 2.21 | 0.75 |
| 14:V:77:VAL:HG23 | 14:V:89:ILE:HG23 | 1.67 | 0.75 |
| 2:B:1440:U:H2' | 2:B:1441:G:H8 | 1.50 | 0.75 |
| 2:B:162:U:H4' | 2:B:163:C:OP1 | 1.84 | 0.75 |
| 2:B:2144:G:O2' | 2:B:2145:C:H5' | 1.86 | 0.75 |
| 8:E:47:LYS:HB3 | 8:E:51:GLU:HB2 | 1.68 | 0.75 |
| 2:B:181:A:H2' | 2:B:182:A:C8 | 2.22 | 0.75 |
| 7:P:91:VAL:HG11 | 7:P:96:LEU:HD11 | 1.67 | 0.75 |
| 8:E:131:THR:HG22 | 8:E:160:ALA:HA | 1.67 | 0.75 |
| 2:B:1178:C:H2' | 2:B:1179:G:C8 | 2.22 | 0.75 |
| 26:F:33:ILE:HB | 26:F:90:LEU:HB2 | 1.69 | 0.75 |
| 2:B:1287:A:H3' | 2:B:1288:G:N2 | 2.02 | 0.75 |
| 13:3:31:ILE:HD11 | 13:3:34:LYS:HD3 | 1.68 | 0.75 |
| 19:H:56:ALA:O | 19:H:60:GLU:HB2 | 1.86 | 0.75 |
| 2:B:1099:G:O4' | 3:I:3:LYS:C | 2.24 | 0.75 |
| 16:L:124:GLY:N | 16:L:143:GLU:HG3 | 2.00 | 0.75 |
| 26:F:33:ILE:HD13 | 26:F:98:PHE:HD2 | 1.49 | 0.75 |
| 4:C:140:VAL:HG12 | 4:C:141:HIS:H | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:1287:A:N7 | 21:N:105:GLY:HA3 | 2.01 | 0.75 |
| 2:B:1872:A:H2' | 2:B:1873:G:O4' | 1.87 | 0.75 |
| 28:R:34:GLU:HG2 | 28:R:60:LYS:HG2 | 1.68 | 0.75 |
| 2:B:743:A:O2' | 2:B:744:U:H5' | 1.87 | 0.75 |
| 2:B:361:G:H2' | 2:B:362:A:H8 | 1.52 | 0.74 |
| 9:Y:2:LYS:HE2 | 9:Y:4:ILE:HD11 | 1.69 | 0.74 |
| 23:Q:26:ALA:HB1 | 23:Q:30:VAL:HB | 1.68 | 0.74 |
| 6:K:112:PHE:O | 6:K:115:ILE:HG22 | 1.86 | 0.74 |
| 5:D:114:LYS:HD2 | 5:D:116:LYS:NZ | 2.02 | 0.74 |
| 10:O:8:THR:HG23 | 10:O:11:LYS:H | 1.51 | 0.74 |
| 23:Q:4:LYS:HZ1 | 23:Q:7:VAL:H | 1.35 | 0.74 |
| 29:T:53:VAL:HG11 | 29:T:87:LEU:HD13 | 1.68 | 0.74 |
| 7:P:91:VAL:HG21 | 7:P:96:LEU:HD21 | 1.70 | 0.74 |
| 26:F:36:ASN:HA | 26:F:87:LYS:HA | 1.67 | 0.74 |
| 12:1:9:LYS:HD3 | 12:1:9:LYS:H | 1.53 | 0.74 |
| 19:H:83:LYS:HB3 | 19:H:149:GLU:HG2 | 1.69 | 0.74 |
| 2:B:631:A:HO2' | 16:L:66:PHE:HD2 | 1.34 | 0.74 |
| 19:H:119:ASN:OD1 | 19:H:121:VAL:HG13 | 1.88 | 0.74 |
| 22:O:12:THR:HG23 | 22:O:16:ARG:HH11 | 1.52 | 0.74 |
| 21:N:33:ILE:HG22 | 21:N:114:GLU:HB2 | 1.68 | 0.74 |
| 21:N:85:PRO:HA | 21:N:88:ALA:HB2 | 1.69 | 0.74 |
| 5:D:148:GLN:HG3 | 5:D:152:PRO:HB3 | 1.69 | 0.74 |
| 9:Y:26:LEU:HB2 | 9:Y:28:LEU:HG | 1.70 | 0.74 |
| 17:M:127:LYS:HD2 | 17:M:127:LYS:H | 1.52 | 0.74 |
| 28:R:28:ALA:O | 28:R:63:VAL:HG21 | 1.87 | 0.74 |
| 2:B:773:U:H5' | 2:B:774:G:OP2 | 1.87 | 0.74 |
| 29:T:29:THR:N | 29:T:91:GLN:HE22 | 1.83 | 0.74 |
| 2:B:1173:U:H2' | 2:B:1174:U:O4' | 1.87 | 0.74 |
| 26:F:87:LYS:HG3 | 26:F:88:VAL:H | 1.52 | 0.74 |
| 22:O:3:LYS:HD3 | 22:O:3:LYS:H | 1.53 | 0.74 |
| 8:E:176:ASP:HB3 | 8:E:179:SER:HB2 | 1.70 | 0.74 |
| 2:B:2355:G:H4' | 31:W:20:LEU:HD13 | 1.67 | 0.74 |
| 2:B:171:U:H2' | 2:B:172:A:C8 | 2.22 | 0.74 |
| 27:G:101:VAL:HG12 | 27:G:115:GLN:HB3 | 1.70 | 0.74 |
| 11:4:2:LYS:HD3 | 11:4:4:ARG:HE | 1.53 | 0.74 |
| 2:B:1484:U:H2' | 2:B:1485:U:C6 | 2.23 | 0.74 |
| 2:B:1387:A:H2' | 2:B:1388:G:H8 | 1.52 | 0.74 |
| 25:U:12:VAL:HG22 | 25:U:69:VAL:HG12 | 1.70 | 0.74 |
| 7:P:56:SER:HB2 | 7:P:75:THR:HG21 | 1.68 | 0.74 |
| 2:B:2591:C:H2' | 2:B:2592:G:H8 | 1.53 | 0.74 |
| 2:B:1485:U:H2' | 2:B:1486:U:C6 | 2.23 | 0.74 |
| 2:B:1935:G:H1' | 2:B:1964:G:N2 | 2.02 | 0.74 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:2800:A:H2' | 2:B:2801:G:O4' | 1.87 | 0.74 |
| 20:J:63:ALA:HA | 20:J:69:ARG:HH12 | 1.51 | 0.74 |
| 2:B:570:G:H2' | 2:B:2030:A:N7 | 2.02 | 0.74 |
| 28:R:4:VAL:O | 28:R:38:VAL:HA | 1.87 | 0.73 |
| 29:T:74:ILE:HG13 | 29:T:75:GLY:H | 1.53 | 0.73 |
| 24:S:27:LYS:O | 24:S:32:ALA:HB2 | 1.88 | 0.73 |
| 23:Q:63:ARG:HH12 | 23:Q:96:ASP:HA | 1.53 | 0.73 |
| 15:2:22:MET:HA | 15:2:28:ARG:HG2 | 1.70 | 0.73 |
| 28:R:4:VAL:HG23 | 28:R:39:LEU:H | 1.52 | 0.73 |
| 2:B:637:A:H5'' | 16:L:112:LEU:HD22 | 1.68 | 0.73 |
| 15:2:33:ARG:HB2 | 15:2:33:ARG:HH21 | 1.53 | 0.73 |
| 5:D:68:PHE:HB3 | 5:D:73:VAL:HG23 | 1.68 | 0.73 |
| 5:D:113:SER:CB | 5:D:168:GLU:H | 2.01 | 0.73 |
| 14:V:40:ILE:H | 14:V:40:ILE:HD13 | 1.54 | 0.73 |
| 2:B:2849:U:H4' | 2:B:2850:A:H5' | 1.71 | 0.73 |
| 8:E:122:GLU:H | 8:E:122:GLU:CD | 1.92 | 0.73 |
| 19:H:18:GLN:HE21 | 19:H:39:ALA:HB1 | 1.52 | 0.73 |
| 6:K:70:ARG:HB3 | 6:K:76:VAL:HG22 | 1.69 | 0.73 |
| 26:F:149:ARG:HH11 | 26:F:149:ARG:HA | 1.53 | 0.73 |
| 25:U:25:LYS:HE3 | 25:U:36:GLU:HG3 | 1.68 | 0.73 |
| 3:I:20:SER:HB3 | 3:I:21:PRO:HD3 | 1.69 | 0.73 |
| 2:B:289:G:H2' | 2:B:290:U:C6 | 2.24 | 0.73 |
| 2:B:2314:A:H1' | 26:F:154:THR:HG21 | 1.70 | 0.73 |
| 23:Q:79:ILE:HA | 23:Q:82:LEU:HD12 | 1.71 | 0.73 |
| 2:B:483:A:H1' | 25:U:56:GLY:HA2 | 1.71 | 0.73 |
| 17:M:59:ARG:HH11 | 17:M:60:GLN:HB3 | 1.51 | 0.73 |
| 2:B:858:G:H21 | 2:B:2268:A:H3' | 1.52 | 0.73 |
| 28:R:24:LYS:HA | 28:R:94:THR:HG23 | 1.71 | 0.73 |
| 26:F:116:LEU:HD23 | 26:F:176:PHE:H | 1.54 | 0.73 |
| 2:B:1440:U:H2' | 2:B:1441:G:C8 | 2.23 | 0.73 |
| 1:A:32:U:H4' | 1:A:52:A:N6 | 2.03 | 0.73 |
| 2:B:1592:C:H2' | 2:B:1593:A:C8 | 2.24 | 0.73 |
| 27:G:89:VAL:HG12 | 27:G:90:GLY:H | 1.51 | 0.73 |
| 2:B:616:A:H3' | 2:B:617:G:H8 | 1.53 | 0.73 |
| 26:F:125:GLY:HA2 | 26:F:162:ASP:HA | 1.70 | 0.73 |
| 26:F:62:GLN:HG3 | 26:F:91:ARG:NH1 | 2.03 | 0.73 |
| 2:B:1203:U:H1' | 16:L:4:ASN:HD21 | 1.52 | 0.73 |
| 17:M:131:VAL:HG12 | 17:M:132:THR:H | 1.54 | 0.73 |
| 23:Q:111:LYS:HB2 | 28:R:48:LYS:NZ | 2.04 | 0.72 |
| 2:B:3:U:H2' | 2:B:4:U:C6 | 2.23 | 0.72 |
| 18:X:21:LEU:HD21 | 18:X:50:VAL:HG11 | 1.70 | 0.72 |
| 2:B:636:G:H3' | 16:L:128:THR:HG21 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 24:S:29:VAL:HA | 24:S:32:ALA:HB3 | 1.71 | 0.72 |
| 24:S:6:LYS:HB2 | 24:S:103:ILE:O | 1.89 | 0.72 |
| 19:H:141:LYS:HD2 | 19:H:141:LYS:N | 2.05 | 0.72 |
| 26:F:134:GLN:HE21 | 26:F:149:ARG:HB2 | 1.53 | 0.72 |
| 31:W:43:LYS:HD2 | 31:W:79:ILE:HD11 | 1.71 | 0.72 |
| 12:1:6:GLU:HB2 | 12:1:52:LYS:NZ | 2.04 | 0.72 |
| 2:B:972:A:H3' | 2:B:973:A:H5'' | 1.70 | 0.72 |
| 7:P:50:ARG:HB2 | 7:P:56:SER:HB3 | 1.72 | 0.72 |
| 14:V:62:THR:HG22 | 14:V:71:LYS:HG2 | 1.71 | 0.72 |
| 2:B:479:A:O2' | 2:B:481:G:H5' | 1.90 | 0.72 |
| 7:P:4:ILE:C | 7:P:6:GLN:H | 1.93 | 0.72 |
| 2:B:664:G:H2' | 2:B:665:U:H6 | 1.54 | 0.72 |
| 2:B:2143:C:H3' | 2:B:2144:G:C8 | 2.24 | 0.72 |
| 2:B:664:G:H2' | 2:B:665:U:C6 | 2.24 | 0.72 |
| 7:P:61:ARG:HB3 | 7:P:61:ARG:HH21 | 1.55 | 0.72 |
| 2:B:455:C:N3 | 2:B:472:A:H2' | 2.05 | 0.72 |
| 19:H:41:LYS:O | 19:H:44:ILE:HG12 | 1.90 | 0.72 |
| 16:L:103:ILE:H | 16:L:103:ILE:HD12 | 1.53 | 0.72 |
| 2:B:1050:A:H2' | 2:B:1051:G:O4' | 1.90 | 0.72 |
| 28:R:58:VAL:HG22 | 28:R:59:ILE:H | 1.54 | 0.72 |
| 23:Q:91:ARG:HE | 23:Q:94:LEU:HD23 | 1.55 | 0.72 |
| 2:B:172:A:H2' | 2:B:173:A:C8 | 2.25 | 0.72 |
| 24:S:20:VAL:O | 24:S:23:LEU:HB2 | 1.90 | 0.72 |
| 2:B:2674:G:H4' | 6:K:30:ARG:HG3 | 1.70 | 0.72 |
| 2:B:192:C:H2' | 2:B:193:U:H5' | 1.72 | 0.72 |
| 2:B:1301:A:O2' | 2:B:1302:A:H2' | 1.90 | 0.72 |
| 26:F:110:ILE:HA | 26:F:111:ARG:CZ | 2.20 | 0.72 |
| 2:B:547:A:H5' | 2:B:548:G:N2 | 2.04 | 0.72 |
| 2:B:2039:U:H2' | 2:B:2040:G:H8 | 1.53 | 0.72 |
| 23:Q:86:SER:HB3 | 28:R:51:VAL:HA | 1.71 | 0.71 |
| 2:B:1060:U:C4 | 2:B:1088:A:N6 | 2.58 | 0.71 |
| 2:B:280:U:H2' | 2:B:281:C:C6 | 2.25 | 0.71 |
| 4:C:128:THR:HA | 4:C:190:THR:HA | 1.72 | 0.71 |
| 14:V:63:ILE:HD13 | 14:V:72:VAL:HG22 | 1.72 | 0.71 |
| 2:B:2502:G:H5' | 2:B:2503:A:C5' | 2.19 | 0.71 |
| 2:B:383:C:H5'' | 2:B:385:C:OP2 | 1.90 | 0.71 |
| 26:F:40:GLY:HA2 | 26:F:84:ILE:HG23 | 1.72 | 0.71 |
| 4:C:80:LEU:HD11 | 4:C:109:LEU:O | 1.90 | 0.71 |
| 2:B:18:U:H2' | 2:B:19:A:H8 | 1.54 | 0.71 |
| 3:I:9:LYS:HG2 | 3:I:57:VAL:HG13 | 1.73 | 0.71 |
| 19:H:46:PHE:HA | 19:H:50:ARG:NH2 | 2.05 | 0.71 |
| 31:W:37:VAL:HG12 | 31:W:38:ARG:N | 2.06 | 0.71 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:3:U:H2' | 2:B:4:U:H6 | 1.56 | 0.71 |
| 2:B:33:C:H2' | 2:B:446:G:N2 | 2.05 | 0.71 |
| 28:R:22:LEU:HD12 | 28:R:25:LEU:HD21 | 1.72 | 0.71 |
| 23:Q:65:ASN:HB2 | 23:Q:75:TYR:HB2 | 1.71 | 0.71 |
| 19:H:115:VAL:HB | 19:H:132:PHE:CD1 | 2.26 | 0.71 |
| 3:I:85:ILE:HD13 | 3:I:137:LEU:HD21 | 1.73 | 0.71 |
| 2:B:1099:G:C5' | 3:I:3:LYS:N | 2.54 | 0.71 |
| 27:G:71:LEU:HA | 27:G:74:MET:SD | 2.31 | 0.71 |
| 6:K:71:ARG:HB3 | 6:K:72:PRO:HD2 | 1.73 | 0.71 |
| 22:O:88:LYS:HE2 | 22:O:116:GLN:HB2 | 1.71 | 0.71 |
| 4:C:103:ILE:HG22 | 4:C:105:ALA:H | 1.54 | 0.71 |
| 21:N:78:LYS:HG3 | 21:N:83:LEU:HG | 1.73 | 0.71 |
| 2:B:2645:G:H3' | 2:B:2646:C:H5' | 1.73 | 0.71 |
| 3:I:105:LEU:HD11 | 3:I:139:VAL:HG21 | 1.70 | 0.71 |
| 11:4:10:LEU:HD12 | 11:4:33:HIS:HA | 1.72 | 0.71 |
| 29:T:69:ARG:HE | 29:T:70:HIS:H | 1.39 | 0.71 |
| 6:K:102:PRO:HA | 6:K:120:PRO:HB3 | 1.70 | 0.71 |
| 18:X:17:GLU:HB3 | 18:X:53:VAL:HG11 | 1.73 | 0.71 |
| 19:H:127:GLU:HA | 19:H:145:ASN:HA | 1.72 | 0.71 |
| 31:W:46:ALA:HB2 | 31:W:78:PHE:HD1 | 1.56 | 0.71 |
| 2:B:2269:G:H4' | 31:W:19:ARG:NH1 | 2.05 | 0.71 |
| 20:J:99:ARG:O | 20:J:103:ILE:HG13 | 1.90 | 0.71 |
| 4:C:233:GLY:H | 4:C:241:LYS:NZ | 1.89 | 0.71 |
| 7:P:7:LEU:H | 7:P:7:LEU:HD12 | 1.56 | 0.70 |
| 2:B:117:G:H5' | 2:B:126:A:H8 | 1.55 | 0.70 |
| 10:O:38:LEU:HB3 | 10:O:41:HIS:NE2 | 2.05 | 0.70 |
| 13:3:18:LYS:HD2 | 13:3:20:GLY:H | 1.56 | 0.70 |
| 20:J:72:LYS:HB2 | 20:J:89:PHE:HB2 | 1.71 | 0.70 |
| 2:B:2756:U:H1' | 2:B:2757:A:H5'' | 1.73 | 0.70 |
| 2:B:1802:A:H2' | 2:B:1803:A:C8 | 2.25 | 0.70 |
| 2:B:1047:G:H1' | 2:B:1110:G:N2 | 2.05 | 0.70 |
| 2:B:370:G:O2' | 2:B:423:A:H3' | 1.91 | 0.70 |
| 20:J:112:GLY:H | 20:J:113:PRO:HD2 | 1.56 | 0.70 |
| 26:F:137:PHE:HB2 | 26:F:138:PRO:HD2 | 1.73 | 0.70 |
| 2:B:1709:U:H2' | 2:B:1710:G:H8 | 1.54 | 0.70 |
| 7:P:50:ARG:CB | 7:P:56:SER:HB3 | 2.21 | 0.70 |
| 30:Z:35:SER:HA | 30:Z:50:ARG:HA | 1.73 | 0.70 |
| 9:Y:6:ILE:O | 9:Y:34:THR:HA | 1.92 | 0.70 |
| 24:S:82:MET:HB2 | 24:S:98:LYS:HB2 | 1.72 | 0.70 |
| 12:1:46:VAL:HG22 | 12:1:47:ILE:H | 1.55 | 0.70 |
| 4:C:20:ASN:HD22 | 4:C:23:LEU:HD13 | 1.56 | 0.70 |
| 2:B:1098:A:H2' | 3:I:4:VAL:CA | 2.22 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 21:N:38:LEU:O | 21:N:42:LYS:HG3 | 1.91 | 0.70 |
| 20:J:45:THR:H | 20:J:46:PRO:HD3 | 1.56 | 0.70 |
| 23:Q:94:LEU:HD12 | 28:R:13:ARG:HB2 | 1.72 | 0.70 |
| 30:Z:5:CYS:HB2 | 30:Z:10:LYS:HB2 | 1.71 | 0.70 |
| 4:C:244:VAL:HB | 4:C:249:VAL:H | 1.56 | 0.70 |
| 18:X:39:GLN:HB3 | 18:X:42:LEU:HD13 | 1.72 | 0.70 |
| 2:B:1024:G:C3' | 2:B:1025:G:H5'' | 2.19 | 0.70 |
| 20:J:37:ARG:NH2 | 20:J:110:PRO:HG3 | 2.07 | 0.70 |
| 2:B:918:A:H2' | 2:B:919:U:H5' | 1.72 | 0.70 |
| 5:D:55:LYS:HB3 | 5:D:60:VAL:HG22 | 1.73 | 0.70 |
| 4:C:57:HIS:CG | 4:C:58:LYS:H | 2.09 | 0.70 |
| 2:B:1124:G:H1' | 11:4:38:GLY:OXT | 1.90 | 0.70 |
| 13:3:22:LYS:HA | 13:3:48:MET:HA | 1.72 | 0.70 |
| 2:B:1856:U:H2' | 2:B:1857:G:H5' | 1.74 | 0.70 |
| 2:B:285:G:H2' | 2:B:286:U:O4' | 1.92 | 0.70 |
| 26:F:64:PRO:HA | 26:F:88:VAL:CG2 | 2.22 | 0.70 |
| 2:B:845:A:C2 | 2:B:847:U:H1' | 2.27 | 0.70 |
| 2:B:919:U:H2' | 2:B:920:A:C8 | 2.27 | 0.70 |
| 1:A:98:G:N1 | 14:V:14:LYS:HB2 | 2.07 | 0.70 |
| 2:B:2144:G:O2' | 2:B:2146:C:H5'' | 1.92 | 0.70 |
| 5:D:113:SER:HB2 | 5:D:168:GLU:H | 1.57 | 0.70 |
| 2:B:2859:G:H2' | 2:B:2860:A:C8 | 2.27 | 0.70 |
| 2:B:2269:G:H4' | 31:W:19:ARG:HH12 | 1.57 | 0.69 |
| 2:B:2353:G:H21 | 31:W:30:VAL:HG22 | 1.57 | 0.69 |
| 2:B:544:C:H2' | 2:B:545:U:C5 | 2.27 | 0.69 |
| 2:B:1552:A:H2' | 2:B:1553:A:H5' | 1.72 | 0.69 |
| 2:B:19:A:H2' | 2:B:20:C:C6 | 2.27 | 0.69 |
| 2:B:2498:C:O2' | 2:B:2499:C:H5' | 1.92 | 0.69 |
| 21:N:97:ILE:HD12 | 21:N:98:LEU:N | 2.07 | 0.69 |
| 2:B:62:U:H3' | 2:B:63:A:C8 | 2.26 | 0.69 |
| 2:B:1082:U:N3 | 2:B:1086:A:C2 | 2.60 | 0.69 |
| 31:W:13:ARG:HG3 | 31:W:14:ASP:H | 1.56 | 0.69 |
| 2:B:2266:A:C4' | 2:B:2267:A:N7 | 2.55 | 0.69 |
| 31:W:49:ASN:HB3 | 31:W:81:ILE:HG12 | 1.74 | 0.69 |
| 16:L:75:ALA:HB2 | 16:L:105:ILE:HG21 | 1.75 | 0.69 |
| 26:F:102:LEU:O | 26:F:103:ILE:HB | 1.93 | 0.69 |
| 2:B:2144:G:N3 | 2:B:2146:C:H5' | 2.07 | 0.69 |
| 19:H:115:VAL:HG22 | 19:H:117:LEU:H | 1.58 | 0.69 |
| 19:H:141:LYS:HD2 | 19:H:141:LYS:H | 1.58 | 0.69 |
| 26:F:45:ASP:HB3 | 26:F:48:LEU:HD22 | 1.73 | 0.69 |
| 2:B:2425:A:H5' | 2:B:2427:C:O4' | 1.91 | 0.69 |
| 2:B:1149:G:H2' | 2:B:1150:C:C6 | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 15:2:19:ARG:HH21 | 15:2:19:ARG:HB3 | 1.57 | 0.69 |
| 25:U:81:ARG:HH21 | 25:U:81:ARG:N | 1.90 | 0.69 |
| 2:B:1785:A:H2' | 2:B:1787:A:N7 | 2.08 | 0.69 |
| 2:B:1346:G:O2' | 2:B:1347:A:H5' | 1.93 | 0.69 |
| 31:W:66:VAL:HA | 31:W:81:ILE:HG22 | 1.74 | 0.69 |
| 27:G:83:THR:HA | 27:G:84:LYS:NZ | 2.08 | 0.69 |
| 17:M:4:PRO:HG2 | 17:M:70:ASP:HA | 1.75 | 0.69 |
| 2:B:2328:A:H2' | 2:B:2329:U:C6 | 2.28 | 0.69 |
| 2:B:1594:U:H2' | 2:B:1595:C:C6 | 2.28 | 0.69 |
| 2:B:580:U:H2' | 2:B:581:C:C6 | 2.28 | 0.69 |
| 2:B:286:U:H2' | 2:B:287:G:C8 | 2.27 | 0.69 |
| 2:B:1406:U:H2' | 2:B:1407:G:C8 | 2.28 | 0.69 |
| 30:Z:27:ARG:HD3 | 30:Z:28:ARG:H | 1.57 | 0.69 |
| 2:B:2336:A:H61 | 31:W:40:ARG:CG | 2.06 | 0.69 |
| 2:B:1081:U:H5' | 3:I:126:ARG:NH1 | 2.08 | 0.69 |
| 2:B:2723:C:H5'' | 21:N:1:MET:HE2 | 1.75 | 0.69 |
| 2:B:165:A:H2' | 2:B:166:U:H6 | 1.58 | 0.69 |
| 26:F:29:ARG:HH11 | 26:F:29:ARG:HB2 | 1.58 | 0.69 |
| 2:B:2867:G:H2' | 2:B:2867:G:N3 | 2.07 | 0.69 |
| 1:A:29:A:H3' | 1:A:30:C:H6 | 1.57 | 0.69 |
| 25:U:87:GLU:OE2 | 25:U:88:ASP:HB2 | 1.92 | 0.68 |
| 29:T:10:VAL:HG21 | 29:T:42:GLU:HG3 | 1.76 | 0.68 |
| 9:Y:4:ILE:HD13 | 9:Y:58:GLU:HA | 1.75 | 0.68 |
| 26:F:64:PRO:HA | 26:F:88:VAL:HG22 | 1.74 | 0.68 |
| 6:K:97:THR:C | 6:K:98:ARG:HE | 1.96 | 0.68 |
| 2:B:704:G:H1' | 2:B:727:A:N6 | 2.09 | 0.68 |
| 23:Q:10:ARG:HA | 23:Q:13:HIS:HB2 | 1.75 | 0.68 |
| 2:B:2471:A:O2' | 2:B:2472:G:H8 | 1.75 | 0.68 |
| 2:B:1486:U:H2' | 2:B:1487:U:H6 | 1.58 | 0.68 |
| 2:B:1469:A:H2' | 2:B:1470:A:C8 | 2.29 | 0.68 |
| 2:B:594:U:H2' | 2:B:595:C:C6 | 2.27 | 0.68 |
| 2:B:1693:U:H1' | 4:C:13:ARG:HH21 | 1.57 | 0.68 |
| 1:A:104:A:H2' | 1:A:105:G:O4' | 1.93 | 0.68 |
| 6:K:18:ARG:HB2 | 6:K:45:GLU:HG3 | 1.74 | 0.68 |
| 20:J:32:LEU:O | 20:J:36:LEU:HD22 | 1.93 | 0.68 |
| 2:B:141:G:H3' | 2:B:141:G:N3 | 2.07 | 0.68 |
| 2:B:30:G:H2' | 2:B:31:C:C6 | 2.28 | 0.68 |
| 17:M:19:GLY:N | 17:M:38:ARG:HH22 | 1.91 | 0.68 |
| 4:C:233:GLY:H | 4:C:241:LYS:HZ1 | 1.41 | 0.68 |
| 2:B:1639:C:H2' | 2:B:1640:A:H5'' | 1.74 | 0.68 |
| 4:C:134:ILE:HD11 | 4:C:163:ILE:HG13 | 1.76 | 0.68 |
| 28:R:38:VAL:O | 28:R:53:PHE:HB3 | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:27:G:HO2' | 2:B:28:A:H8 | 1.41 | 0.68 |
| 27:G:120:ILE:HD11 | 27:G:132:LEU:HB2 | 1.75 | 0.68 |
| 2:B:543:G:H21 | 2:B:545:U:H5' | 1.58 | 0.68 |
| 22:O:67:ASN:H | 22:O:70:ALA:HB3 | 1.58 | 0.68 |
| 2:B:1230:A:H2' | 2:B:1231:U:C6 | 2.28 | 0.68 |
| 28:R:76:LYS:HB2 | 28:R:85:LYS:HB2 | 1.76 | 0.68 |
| 8:E:136:GLN:HE22 | 8:E:139:LYS:HD3 | 1.59 | 0.68 |
| 31:W:23:LYS:NZ | 31:W:24:ARG:HG3 | 2.09 | 0.68 |
| 20:J:25:LEU:HD22 | 20:J:26:GLY:H | 1.58 | 0.68 |
| 2:B:704:G:H1' | 2:B:727:A:H61 | 1.58 | 0.68 |
| 29:T:44:LYS:O | 29:T:48:GLN:HG2 | 1.94 | 0.68 |
| 2:B:2895:G:H2' | 2:B:2896:C:C6 | 2.28 | 0.68 |
| 2:B:1335:C:H2' | 2:B:1336:A:H8 | 1.58 | 0.68 |
| 31:W:65:LYS:HD2 | 31:W:84:GLU:HB3 | 1.74 | 0.68 |
| 2:B:27:G:H1' | 2:B:513:A:N6 | 2.09 | 0.68 |
| 26:F:34:THR:HA | 26:F:89:THR:HG22 | 1.76 | 0.68 |
| 2:B:2039:U:H2' | 2:B:2040:G:C8 | 2.29 | 0.68 |
| 2:B:1164:C:H2' | 2:B:1165:A:H8 | 1.59 | 0.68 |
| 2:B:2267:A:H5'' | 2:B:2268:A:H5' | 1.74 | 0.68 |
| 2:B:1812:U:H1' | 4:C:43:ASN:ND2 | 2.07 | 0.68 |
| 2:B:2769:U:H2' | 2:B:2770:G:C8 | 2.27 | 0.68 |
| 31:W:74:LYS:HE2 | 31:W:74:LYS:HA | 1.76 | 0.68 |
| 27:G:84:LYS:HB2 | 27:G:132:LEU:H | 1.57 | 0.68 |
| 2:B:2886:A:H62 | 10:O:39:ARG:CZ | 2.06 | 0.68 |
| 2:B:1550:C:H2' | 2:B:1551:A:H8 | 1.59 | 0.68 |
| 2:B:137:U:H2' | 2:B:138:U:O4' | 1.94 | 0.68 |
| 2:B:982:C:O2 | 2:B:982:C:H5' | 1.94 | 0.68 |
| 2:B:2741:A:H2' | 2:B:2742:G:O4' | 1.94 | 0.68 |
| 8:E:3:LEU:HB2 | 8:E:12:LEU:HB2 | 1.76 | 0.68 |
| 16:L:90:VAL:HB | 16:L:122:VAL:HG12 | 1.76 | 0.67 |
| 4:C:144:GLU:HG3 | 4:C:151:GLY:N | 2.09 | 0.67 |
| 5:D:27:ILE:HG23 | 5:D:201:LEU:HD12 | 1.76 | 0.67 |
| 2:B:1060:U:O2 | 2:B:1088:A:N7 | 2.27 | 0.67 |
| 2:B:2071:A:H2' | 2:B:2072:C:C6 | 2.29 | 0.67 |
| 22:O:15:ARG:HH21 | 22:O:95:SER:CB | 2.06 | 0.67 |
| 2:B:423:A:H5' | 2:B:424:G:H5'' | 1.76 | 0.67 |
| 1:A:2:G:H2' | 1:A:3:C:C6 | 2.29 | 0.67 |
| 2:B:165:A:H2' | 2:B:166:U:C6 | 2.30 | 0.67 |
| 4:C:156:SER:O | 4:C:194:VAL:HG11 | 1.93 | 0.67 |
| 2:B:2331:G:O2' | 31:W:40:ARG:HB2 | 1.95 | 0.67 |
| 4:C:180:MET:HB2 | 4:C:268:ARG:HB2 | 1.76 | 0.67 |
| 2:B:140:C:H4' | 2:B:141:G:C6 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 6:K:118:LEU:O | 6:K:120:PRO:HD2 | 1.94 | 0.67 |
| 18:X:49:ASP:O | 18:X:53:VAL:HG23 | 1.95 | 0.67 |
| 21:N:96:ARG:HH11 | 21:N:116:VAL:HG23 | 1.60 | 0.67 |
| 2:B:2804:U:H2' | 2:B:2805:C:C6 | 2.29 | 0.67 |
| 2:B:1437:C:H2' | 2:B:1438:U:H6 | 1.59 | 0.67 |
| 28:R:14:VAL:HG21 | 28:R:98:ILE:HG12 | 1.75 | 0.67 |
| 2:B:1386:C:H2' | 2:B:1387:A:C8 | 2.30 | 0.67 |
| 2:B:423:A:H5' | 2:B:424:G:C5' | 2.24 | 0.67 |
| 2:B:857:G:O2' | 2:B:858:G:H5' | 1.95 | 0.67 |
| 11:4:7:VAL:HG23 | 11:4:35:GLN:HB2 | 1.76 | 0.67 |
| 17:M:64:TRP:HB2 | 17:M:104:GLU:HB2 | 1.76 | 0.67 |
| 2:B:720:U:H2' | 2:B:721:A:C8 | 2.29 | 0.67 |
| 26:F:62:GLN:HE21 | 26:F:91:ARG:NH1 | 1.92 | 0.67 |
| 15:2:31:LEU:HD22 | 15:2:42:LEU:HD12 | 1.76 | 0.67 |
| 2:B:992:C:H4' | 28:R:74:ILE:HD13 | 1.76 | 0.67 |
| 8:E:5:LEU:HD22 | 8:E:122:GLU:HG3 | 1.77 | 0.67 |
| 27:G:25:ILE:HG22 | 27:G:78:VAL:HG11 | 1.77 | 0.67 |
| 27:G:84:LYS:CB | 27:G:132:LEU:H | 2.08 | 0.67 |
| 21:N:34:ILE:HB | 21:N:113:ILE:HG22 | 1.76 | 0.67 |
| 18:X:56:LEU:O | 18:X:57:LEU:HB2 | 1.93 | 0.67 |
| 2:B:460:A:H2' | 2:B:461:C:O4' | 1.94 | 0.67 |
| 2:B:1429:G:H2' | 2:B:1430:G:H8 | 1.60 | 0.67 |
| 2:B:2213:U:O2 | 2:B:2213:U:H2' | 1.95 | 0.67 |
| 6:K:35:VAL:HG12 | 6:K:69:VAL:HG22 | 1.77 | 0.67 |
| 20:J:12:LYS:HD2 | 20:J:41:LYS:HD3 | 1.77 | 0.67 |
| 2:B:1175:A:C3' | 2:B:1176:U:H5' | 2.23 | 0.67 |
| 3:I:73:PRO:HG2 | 3:I:78:LEU:HD21 | 1.75 | 0.67 |
| 21:N:72:ASP:O | 21:N:75:ILE:HG13 | 1.95 | 0.67 |
| 24:S:20:VAL:HG23 | 24:S:23:LEU:HD12 | 1.77 | 0.67 |
| 2:B:609:A:H2' | 2:B:610:C:O4' | 1.95 | 0.67 |
| 28:R:31:GLU:H | 28:R:63:VAL:HG22 | 1.58 | 0.67 |
| 2:B:796:C:H2' | 2:B:797:G:H8 | 1.60 | 0.67 |
| 31:W:48:ALA:HB3 | 31:W:81:ILE:HG13 | 1.77 | 0.67 |
| 5:D:37:VAL:HG23 | 5:D:91:THR:HA | 1.77 | 0.67 |
| 23:Q:63:ARG:HH12 | 23:Q:96:ASP:HB2 | 1.58 | 0.66 |
| 23:Q:63:ARG:HH22 | 23:Q:96:ASP:CA | 2.06 | 0.66 |
| 17:M:43:ALA:O | 17:M:46:ILE:HG12 | 1.95 | 0.66 |
| 2:B:2146:C:H4' | 2:B:2148:G:N7 | 2.10 | 0.66 |
| 12:1:26:LYS:HD3 | 12:1:52:LYS:HB3 | 1.77 | 0.66 |
| 6:K:70:ARG:HB3 | 6:K:76:VAL:HG13 | 1.76 | 0.66 |
| 2:B:718:A:H3' | 2:B:719:C:H6 | 1.61 | 0.66 |
| 2:B:2872:A:O2' | 2:B:2873:A:H5'' | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:2352:A:C6 | 31:W:30:VAL:HG11 | 2.30 | 0.66 |
| 14:V:35:GLU:HG3 | 14:V:93:ARG:CZ | 2.25 | 0.66 |
| 26:F:90:LEU:HB3 | 26:F:95:MET:HA | 1.77 | 0.66 |
| 2:B:2265:U:H3' | 2:B:2266:A:H5'' | 1.76 | 0.66 |
| 8:E:29:HIS:NE2 | 16:L:8:PRO:HG3 | 2.10 | 0.66 |
| 15:2:35:ARG:HG3 | 15:2:42:LEU:HD21 | 1.75 | 0.66 |
| 2:B:2142:A:H2' | 2:B:2143:C:O4' | 1.96 | 0.66 |
| 2:B:2149:U:H2' | 2:B:2150:C:C6 | 2.30 | 0.66 |
| 2:B:1693:U:H1' | 4:C:13:ARG:NH2 | 2.11 | 0.66 |
| 5:D:178:VAL:HB | 5:D:188:LEU:HB2 | 1.78 | 0.66 |
| 26:F:76:PHE:HD2 | 26:F:78:ILE:HD13 | 1.59 | 0.66 |
| 26:F:104:THR:C | 26:F:108:PRO:HG2 | 2.16 | 0.66 |
| 2:B:1655:A:H5' | 5:D:118:PHE:HB2 | 1.76 | 0.66 |
| 29:T:73:ARG:HH21 | 29:T:73:ARG:HB3 | 1.58 | 0.66 |
| 22:O:24:THR:HG23 | 22:O:90:VAL:HG12 | 1.77 | 0.66 |
| 2:B:2353:G:N3 | 31:W:30:VAL:HG13 | 2.10 | 0.66 |
| 5:D:29:VAL:O | 5:D:185:ASN:HB3 | 1.95 | 0.66 |
| 14:V:30:ILE:HA | 14:V:91:PHE:O | 1.96 | 0.66 |
| 26:F:101:ARG:CZ | 26:F:138:PRO:HB2 | 2.26 | 0.66 |
| 2:B:1550:C:H2' | 2:B:1551:A:C8 | 2.30 | 0.66 |
| 6:K:43:ILE:HG21 | 6:K:46:ALA:HB2 | 1.77 | 0.66 |
| 12:1:33:LEU:HB3 | 12:1:51:ALA:HB3 | 1.77 | 0.66 |
| 25:U:20:LYS:HB2 | 25:U:20:LYS:HZ3 | 1.59 | 0.66 |
| 2:B:581:C:H2' | 2:B:582:A:C8 | 2.30 | 0.66 |
| 2:B:1579:A:H2' | 2:B:1580:A:C8 | 2.30 | 0.66 |
| 2:B:1716:U:H2' | 2:B:1717:A:H8 | 1.60 | 0.66 |
| 2:B:1726:C:H2' | 2:B:1727:C:C6 | 2.30 | 0.66 |
| 14:V:4:ILE:HB | 14:V:63:ILE:HG13 | 1.78 | 0.66 |
| 5:D:8:LYS:HG2 | 5:D:197:THR:H | 1.60 | 0.66 |
| 21:N:80:PHE:O | 21:N:85:PRO:HD3 | 1.96 | 0.66 |
| 27:G:167:VAL:HG23 | 27:G:168:VAL:H | 1.59 | 0.66 |
| 2:B:2360:G:H4' | 16:L:61:LEU:HD11 | 1.76 | 0.66 |
| 16:L:90:VAL:HB | 16:L:122:VAL:HA | 1.75 | 0.66 |
| 8:E:29:HIS:HA | 8:E:32:VAL:HG22 | 1.78 | 0.66 |
| 3:I:126:ARG:HH11 | 3:I:126:ARG:HB3 | 1.60 | 0.66 |
| 2:B:1486:U:H2' | 2:B:1487:U:C6 | 2.31 | 0.66 |
| 2:B:1796:U:H2' | 2:B:1797:G:H8 | 1.60 | 0.66 |
| 2:B:2102:G:H2' | 2:B:2103:C:O4' | 1.95 | 0.66 |
| 2:B:2861:U:H2' | 2:B:2862:G:H8 | 1.60 | 0.66 |
| 31:W:51:GLY:HA3 | 31:W:59:PHE:CB | 2.26 | 0.66 |
| 19:H:31:VAL:O | 19:H:33:GLN:N | 2.29 | 0.66 |
| 2:B:2885:G:H2' | 2:B:2886:A:O4' | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 30:Z:71:LEU:HD12 | 30:Z:76:GLU:HG2 | 1.77 | 0.66 |
| 27:G:93:TYR:O | 27:G:94:ARG:HG3 | 1.96 | 0.66 |
| 10:0:43:THR:HG23 | 10:0:47:TYR:O | 1.96 | 0.66 |
| 2:B:2893:A:H5'' | 2:B:2894:G:H5' | 1.76 | 0.66 |
| 2:B:729:G:H2' | 2:B:1775:U:H1' | 1.76 | 0.66 |
| 2:B:365:U:H2' | 2:B:366:C:C6 | 2.31 | 0.66 |
| 25:U:40:LEU:HA | 25:U:60:LYS:O | 1.96 | 0.66 |
| 16:L:65:GLY:O | 16:L:66:PHE:HB2 | 1.95 | 0.66 |
| 2:B:1709:U:H2' | 2:B:1710:G:C8 | 2.31 | 0.66 |
| 2:B:2137:U:H2' | 2:B:2138:G:O4' | 1.96 | 0.66 |
| 8:E:194:LYS:O | 8:E:197:GLU:HB3 | 1.96 | 0.66 |
| 2:B:233:A:H61 | 2:B:428:A:N6 | 1.92 | 0.66 |
| 4:C:81:GLU:HB2 | 4:C:90:ILE:HG22 | 1.78 | 0.66 |
| 24:S:66:ILE:HA | 24:S:69:LEU:HD22 | 1.77 | 0.66 |
| 8:E:88:ARG:O | 8:E:90:GLN:HG3 | 1.96 | 0.66 |
| 8:E:143:LEU:HB3 | 8:E:146:VAL:HG21 | 1.78 | 0.66 |
| 15:2:26:ASN:O | 15:2:30:VAL:HG23 | 1.95 | 0.66 |
| 2:B:18:U:H2' | 2:B:19:A:C8 | 2.30 | 0.66 |
| 2:B:713:G:H21 | 2:B:718:A:H2 | 1.43 | 0.66 |
| 4:C:173:LEU:HD13 | 4:C:173:LEU:H | 1.60 | 0.66 |
| 2:B:351:C:H2' | 2:B:352:A:C8 | 2.32 | 0.65 |
| 11:4:3:VAL:HG23 | 11:4:4:ARG:H | 1.61 | 0.65 |
| 2:B:1283:G:N2 | 2:B:1286:A:H5' | 2.11 | 0.65 |
| 2:B:2557:G:H2' | 2:B:2558:C:C6 | 2.31 | 0.65 |
| 3:I:1:ALA:HB1 | 3:I:2:LYS:HD2 | 1.77 | 0.65 |
| 31:W:18:LYS:HA | 31:W:18:LYS:HE3 | 1.77 | 0.65 |
| 21:N:72:ASP:HB3 | 21:N:75:ILE:HG12 | 1.78 | 0.65 |
| 24:S:74:ILE:HD13 | 24:S:105:VAL:HG22 | 1.78 | 0.65 |
| 2:B:2795:C:H2' | 2:B:2796:U:O4' | 1.97 | 0.65 |
| 2:B:1381:G:H2' | 2:B:1382:G:H5' | 1.78 | 0.65 |
| 2:B:825:A:H1' | 16:L:54:GLN:NE2 | 2.12 | 0.65 |
| 25:U:39:ASN:HB3 | 25:U:62:ALA:HB3 | 1.79 | 0.65 |
| 20:J:57:LEU:HD21 | 20:J:128:ASN:HA | 1.77 | 0.65 |
| 3:I:123:ALA:HA | 3:I:126:ARG:HH12 | 1.61 | 0.65 |
| 14:V:66:ASP:HB3 | 14:V:68:LYS:HE2 | 1.79 | 0.65 |
| 24:S:17:VAL:C | 24:S:19:LEU:H | 1.98 | 0.65 |
| 2:B:1354:A:H2' | 2:B:1355:G:O4' | 1.97 | 0.65 |
| 27:G:10:VAL:HG21 | 27:G:47:ASN:O | 1.97 | 0.65 |
| 6:K:41:ILE:HG13 | 6:K:42:THR:H | 1.61 | 0.65 |
| 16:L:79:LEU:HB2 | 16:L:113:ALA:HB3 | 1.77 | 0.65 |
| 12:1:7:LYS:HD2 | 13:3:33:THR:HG21 | 1.78 | 0.65 |
| 2:B:1843:C:H5'' | 4:C:250:GLN:HE21 | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2892:G:H5'' | 2:B:2894:G:N2 | 2.11 | 0.65 |
| 2:B:419:U:H2' | 2:B:420:C:C6 | 2.31 | 0.65 |
| 5:D:14:ILE:HG23 | 5:D:22:ILE:HB | 1.76 | 0.65 |
| 27:G:17:LYS:HZ2 | 27:G:17:LYS:HA | 1.60 | 0.65 |
| 2:B:1174:U:H4' | 2:B:1176:U:H1' | 1.77 | 0.65 |
| 17:M:40:ARG:HB2 | 17:M:93:VAL:CG2 | 2.27 | 0.65 |
| 2:B:138:U:H2' | 2:B:140:C:N1 | 2.12 | 0.65 |
| 2:B:2143:C:H2' | 2:B:2144:G:O4' | 1.97 | 0.65 |
| 17:M:67:VAL:HG11 | 17:M:102:LEU:HD13 | 1.77 | 0.65 |
| 2:B:254:G:H22 | 13:3:7:ARG:HH21 | 1.44 | 0.65 |
| 2:B:589:U:H2' | 2:B:590:A:C8 | 2.31 | 0.65 |
| 2:B:2788:C:H2' | 2:B:2789:C:C6 | 2.32 | 0.65 |
| 2:B:1788:C:O2' | 2:B:1789:A:H5' | 1.96 | 0.65 |
| 2:B:1080:A:H2' | 2:B:1081:U:C6 | 2.30 | 0.65 |
| 20:J:98:GLU:H | 20:J:98:GLU:CD | 2.00 | 0.65 |
| 12:1:43:ARG:HH21 | 12:1:43:ARG:HB3 | 1.61 | 0.65 |
| 4:C:141:HIS:CG | 4:C:142:ASN:H | 2.15 | 0.65 |
| 5:D:53:GLY:HA3 | 5:D:77:ARG:HG3 | 1.77 | 0.65 |
| 26:F:102:LEU:HA | 26:F:106:ALA:HB3 | 1.79 | 0.65 |
| 5:D:34:VAL:CG1 | 5:D:94:GLN:H | 2.09 | 0.65 |
| 2:B:1203:U:H3' | 2:B:1204:A:C5' | 2.27 | 0.65 |
| 12:1:36:LYS:HG2 | 12:1:47:ILE:HG13 | 1.79 | 0.65 |
| 2:B:947:A:HO2' | 2:B:984:A:H2 | 1.45 | 0.65 |
| 7:P:46:VAL:HA | 7:P:60:VAL:HG12 | 1.79 | 0.65 |
| 2:B:654:A:H2' | 2:B:655:A:H5'' | 1.77 | 0.65 |
| 23:Q:63:ARG:NH1 | 23:Q:96:ASP:HA | 2.11 | 0.65 |
| 5:D:10:GLY:HA3 | 5:D:26:VAL:N | 2.07 | 0.65 |
| 27:G:140:ILE:HA | 27:G:143:VAL:HG22 | 1.79 | 0.65 |
| 2:B:495:G:H21 | 24:S:61:ASN:ND2 | 1.92 | 0.65 |
| 2:B:2646:C:OP2 | 2:B:2732:G:H2' | 1.97 | 0.65 |
| 25:U:11:ILE:HG22 | 25:U:70:ALA:HB3 | 1.79 | 0.65 |
| 21:N:114:GLU:HG2 | 21:N:115:LEU:N | 2.12 | 0.65 |
| 2:B:1786:A:H1' | 2:B:1938:A:N6 | 2.12 | 0.65 |
| 2:B:1412:U:H2' | 2:B:1413:A:C8 | 2.32 | 0.65 |
| 2:B:2109:U:H2' | 2:B:2180:U:H3 | 1.62 | 0.65 |
| 2:B:38:A:O2' | 8:E:43:THR:HA | 1.97 | 0.65 |
| 6:K:35:VAL:HG23 | 6:K:36:GLY:N | 2.07 | 0.65 |
| 17:M:40:ARG:HD3 | 17:M:93:VAL:HG21 | 1.79 | 0.65 |
| 2:B:150:U:H2' | 2:B:151:C:C6 | 2.32 | 0.65 |
| 2:B:1515:A:H2' | 2:B:1516:G:O4' | 1.97 | 0.65 |
| 28:R:39:LEU:HB3 | 28:R:53:PHE:HA | 1.78 | 0.65 |
| 14:V:77:VAL:HG12 | 17:M:136:MET:HG2 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:I:27:LEU:HD12 | 3:I:32:VAL:HG11 | 1.77 | 0.65 |
| 2:B:721:A:H2' | 2:B:722:A:C8 | 2.32 | 0.65 |
| 2:B:1381:G:C2' | 2:B:1382:G:H5' | 2.26 | 0.65 |
| 2:B:1507:C:H2' | 2:B:1508:A:H4' | 1.79 | 0.65 |
| 2:B:96:C:H4' | 18:X:41:HIS:ND1 | 2.12 | 0.65 |
| 2:B:2461:A:H2' | 2:B:2462:C:C6 | 2.32 | 0.65 |
| 22:O:53:THR:HB | 22:O:65:THR:HG22 | 1.79 | 0.65 |
| 23:Q:107:ALA:HB1 | 28:R:48:LYS:HE2 | 1.78 | 0.64 |
| 19:H:2:GLN:O | 19:H:3:VAL:HG22 | 1.98 | 0.64 |
| 14:V:44:HIS:NE2 | 14:V:85:LYS:HB2 | 2.11 | 0.64 |
| 24:S:6:LYS:HB3 | 24:S:104:THR:HG23 | 1.79 | 0.64 |
| 8:E:189:THR:O | 8:E:193:VAL:HG23 | 1.97 | 0.64 |
| 2:B:2799:A:H4' | 2:B:2800:A:O4' | 1.97 | 0.64 |
| 2:B:2798:U:H1' | 2:B:2800:A:N6 | 2.11 | 0.64 |
| 2:B:528:A:C2 | 2:B:2042:A:H2' | 2.32 | 0.64 |
| 2:B:717:C:H3' | 2:B:718:A:H5'' | 1.77 | 0.64 |
| 22:O:56:LYS:O | 22:O:60:GLU:HG2 | 1.97 | 0.64 |
| 2:B:1268:A:H2' | 2:B:1269:A:O4' | 1.97 | 0.64 |
| 2:B:275:C:H2' | 2:B:276:U:O4' | 1.97 | 0.64 |
| 26:F:168:LEU:HD13 | 26:F:169:LEU:N | 2.12 | 0.64 |
| 2:B:974:G:OP2 | 28:R:78:ARG:HD3 | 1.97 | 0.64 |
| 21:N:37:THR:HB | 21:N:40:LYS:HG3 | 1.80 | 0.64 |
| 2:B:2579:C:H1' | 5:D:130:GLN:NE2 | 2.05 | 0.64 |
| 20:J:43:GLU:O | 20:J:45:THR:N | 2.30 | 0.64 |
| 3:I:72:THR:HG22 | 3:I:115:ASP:OD2 | 1.97 | 0.64 |
| 4:C:77:VAL:HG23 | 4:C:112:GLY:H | 1.62 | 0.64 |
| 2:B:1485:U:H2' | 2:B:1486:U:H6 | 1.61 | 0.64 |
| 2:B:1164:C:H2' | 2:B:1165:A:C8 | 2.33 | 0.64 |
| 2:B:222:A:N6 | 2:B:232:G:H1' | 2.13 | 0.64 |
| 2:B:417:C:H2' | 2:B:418:C:C6 | 2.33 | 0.64 |
| 5:D:107:VAL:HG13 | 5:D:203:VAL:HG23 | 1.79 | 0.64 |
| 14:V:79:ARG:HA | 14:V:86:LEU:HA | 1.78 | 0.64 |
| 2:B:78:U:H2' | 2:B:79:C:C6 | 2.33 | 0.64 |
| 17:M:71:LYS:HD3 | 17:M:95:LEU:HD13 | 1.80 | 0.64 |
| 2:B:1439:A:C6 | 2:B:1552:A:N7 | 2.65 | 0.64 |
| 2:B:126:A:H5' | 15:2:19:ARG:CG | 2.28 | 0.64 |
| 9:Y:28:LEU:HA | 9:Y:33:HIS:HD2 | 1.62 | 0.64 |
| 2:B:592:A:H2' | 2:B:593:U:C6 | 2.32 | 0.64 |
| 26:F:41:GLU:O | 26:F:43:ILE:HG22 | 1.97 | 0.64 |
| 2:B:460:A:P | 15:2:41:ARG:HH12 | 2.20 | 0.64 |
| 2:B:2243:U:H2' | 2:B:2244:U:C6 | 2.32 | 0.64 |
| 2:B:1939:U:H6 | 2:B:1939:U:H5' | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 29:T:39:THR:HG22 | 29:T:42:GLU:HG2 | 1.80 | 0.64 |
| 2:B:564:C:O2' | 2:B:565:C:H5' | 1.98 | 0.64 |
| 3:I:41:PHE:O | 3:I:45:THR:HG23 | 1.98 | 0.64 |
| 5:D:62:LYS:HD2 | 5:D:62:LYS:H | 1.61 | 0.64 |
| 28:R:78:ARG:HB3 | 28:R:83:TYR:HB3 | 1.79 | 0.64 |
| 4:C:159:THR:O | 4:C:194:VAL:HG12 | 1.97 | 0.64 |
| 30:Z:39:TRP:NE1 | 30:Z:41:GLU:HG2 | 2.12 | 0.64 |
| 2:B:1916:A:H2' | 2:B:1917:U:O4' | 1.98 | 0.64 |
| 7:P:50:ARG:HB3 | 7:P:57:ALA:N | 2.13 | 0.64 |
| 18:X:10:SER:H | 18:X:60:LYS:HE2 | 1.60 | 0.64 |
| 26:F:177:ARG:CZ | 26:F:177:ARG:HA | 2.28 | 0.64 |
| 4:C:144:GLU:HG3 | 4:C:151:GLY:H | 1.62 | 0.64 |
| 26:F:105:ILE:C | 26:F:108:PRO:HD2 | 2.18 | 0.64 |
| 5:D:34:VAL:HB | 5:D:48:ILE:HD11 | 1.80 | 0.64 |
| 2:B:784:G:H5'' | 4:C:225:ASN:OD1 | 1.97 | 0.64 |
| 2:B:278:A:N3 | 2:B:278:A:H2' | 2.12 | 0.64 |
| 20:J:16:TYR:O | 20:J:55:ILE:HG12 | 1.97 | 0.64 |
| 2:B:2897:U:H2' | 2:B:2898:U:C6 | 2.33 | 0.64 |
| 2:B:590:A:H2' | 2:B:591:U:C6 | 2.32 | 0.64 |
| 2:B:2241:A:H2' | 2:B:2242:G:C8 | 2.33 | 0.64 |
| 2:B:2649:C:H2' | 2:B:2650:U:H6 | 1.63 | 0.64 |
| 14:V:44:HIS:HE1 | 14:V:86:LEU:H | 1.46 | 0.64 |
| 26:F:31:GLU:O | 26:F:32:LYS:HD3 | 1.98 | 0.64 |
| 2:B:2330:G:H21 | 31:W:38:ARG:HA | 1.61 | 0.64 |
| 30:Z:76:GLU:HG3 | 30:Z:77:LYS:N | 2.13 | 0.64 |
| 2:B:2150:C:H2' | 2:B:2151:U:C6 | 2.32 | 0.64 |
| 2:B:1372:U:H4' | 2:B:2213:U:O2 | 1.98 | 0.64 |
| 2:B:315:G:H2' | 2:B:316:C:C6 | 2.33 | 0.64 |
| 2:B:634:C:H2' | 2:B:635:C:H6 | 1.63 | 0.64 |
| 4:C:128:THR:HG23 | 4:C:190:THR:HG22 | 1.80 | 0.64 |
| 14:V:44:HIS:CE1 | 14:V:86:LEU:H | 2.15 | 0.64 |
| 2:B:2312:U:O2 | 26:F:38:GLY:HA3 | 1.98 | 0.64 |
| 2:B:1406:U:H2' | 2:B:1407:G:H8 | 1.63 | 0.64 |
| 4:C:264:LYS:HG3 | 4:C:265:PHE:HD2 | 1.63 | 0.64 |
| 2:B:1098:A:H3' | 3:I:3:LYS:CB | 2.26 | 0.64 |
| 26:F:72:SER:HA | 26:F:78:ILE:HG22 | 1.79 | 0.64 |
| 4:C:80:LEU:HD21 | 4:C:109:LEU:HB2 | 1.80 | 0.64 |
| 2:B:2529:G:H5'' | 27:G:174:LYS:HB2 | 1.79 | 0.64 |
| 2:B:1019:U:H2' | 2:B:1020:A:H8 | 1.63 | 0.64 |
| 2:B:181:A:H2' | 2:B:182:A:H8 | 1.62 | 0.64 |
| 4:C:14:HIS:O | 4:C:203:VAL:HG11 | 1.97 | 0.64 |
| 2:B:1599:U:H2' | 2:B:1600:C:C6 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 6:K:85:VAL:O | 6:K:87:LEU:HD23 | 1.98 | 0.64 |
| 2:B:898:C:C2' | 2:B:899:A:H5'' | 2.28 | 0.64 |
| 2:B:857:G:C2' | 2:B:858:G:H5' | 2.28 | 0.63 |
| 29:T:55:VAL:HG13 | 29:T:85:VAL:HG12 | 1.79 | 0.63 |
| 7:P:4:ILE:HG22 | 7:P:5:LYS:N | 2.12 | 0.63 |
| 2:B:281:C:H2' | 2:B:282:A:H8 | 1.63 | 0.63 |
| 1:A:43:C:O2' | 26:F:91:ARG:HD2 | 1.98 | 0.63 |
| 2:B:899:A:H2' | 2:B:900:A:O4' | 1.98 | 0.63 |
| 2:B:307:G:N2 | 2:B:309:A:H3' | 2.14 | 0.63 |
| 2:B:2064:C:H2' | 2:B:2065:C:C6 | 2.33 | 0.63 |
| 11:4:15:LYS:O | 11:4:16:ILE:HB | 1.99 | 0.63 |
| 16:L:55:MET:HE2 | 16:L:56:PRO:HD2 | 1.79 | 0.63 |
| 2:B:1100:C:OP2 | 3:I:2:LYS:HB3 | 1.98 | 0.63 |
| 31:W:39:GLN:HG3 | 31:W:42:THR:HB | 1.80 | 0.63 |
| 19:H:31:VAL:O | 19:H:32:PRO:C | 2.36 | 0.63 |
| 2:B:1176:U:H2' | 2:B:1177:G:C8 | 2.34 | 0.63 |
| 3:I:25:PRO:O | 3:I:29:GLN:HG3 | 1.97 | 0.63 |
| 3:I:42:ASN:HA | 3:I:45:THR:OG1 | 1.97 | 0.63 |
| 8:E:188:MET:HG2 | 8:E:193:VAL:HG22 | 1.80 | 0.63 |
| 2:B:876:C:H3' | 2:B:877:A:C8 | 2.33 | 0.63 |
| 2:B:2078:C:H2' | 2:B:2079:U:C6 | 2.33 | 0.63 |
| 21:N:79:LEU:HA | 21:N:83:LEU:HD12 | 1.80 | 0.63 |
| 2:B:1853:A:N1 | 2:B:2087:G:H1' | 2.13 | 0.63 |
| 4:C:123:ILE:HD13 | 4:C:135:PRO:HG2 | 1.80 | 0.63 |
| 2:B:2455:G:H2' | 2:B:2456:C:C6 | 2.34 | 0.63 |
| 2:B:2008:C:H2' | 2:B:2009:A:H8 | 1.62 | 0.63 |
| 2:B:2052:A:OP1 | 5:D:145:SER:HA | 1.98 | 0.63 |
| 2:B:2803:G:H2' | 2:B:2804:U:H6 | 1.63 | 0.63 |
| 2:B:947:A:H2' | 2:B:948:C:C6 | 2.34 | 0.63 |
| 8:E:31:VAL:HG21 | 8:E:104:ALA:HB2 | 1.80 | 0.63 |
| 22:O:11:ALA:HB2 | 22:O:96:GLY:N | 2.13 | 0.63 |
| 14:V:80:HIS:HD2 | 14:V:82:TYR:H | 1.43 | 0.63 |
| 26:F:141:ASP:O | 26:F:145:VAL:HG13 | 1.99 | 0.63 |
| 16:L:70:LYS:O | 16:L:73:ILE:HG12 | 1.98 | 0.63 |
| 2:B:2443:C:O2' | 2:B:2444:G:H5' | 1.97 | 0.63 |
| 3:I:121:ILE:HD13 | 3:I:121:ILE:N | 2.13 | 0.63 |
| 25:U:81:ARG:H | 25:U:81:ARG:NH2 | 1.95 | 0.63 |
| 2:B:580:U:H2' | 2:B:581:C:H6 | 1.62 | 0.63 |
| 2:B:967:U:H2' | 2:B:968:C:C6 | 2.33 | 0.63 |
| 2:B:394:C:O2' | 2:B:395:U:H5' | 1.99 | 0.63 |
| 23:Q:60:TRP:O | 23:Q:63:ARG:HG3 | 1.99 | 0.63 |
| 19:H:9:VAL:HB | 19:H:13:GLY:HA3 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 6:K:19:VAL:HG12 | 6:K:43:ILE:HA | 1.79 | 0.63 |
| 25:U:65:GLN:HB2 | 25:U:68:ASN:ND2 | 2.13 | 0.63 |
| 21:N:25:ALA:HB1 | 21:N:48:VAL:HG13 | 1.79 | 0.63 |
| 2:B:2722:G:H4' | 21:N:4:ARG:HB2 | 1.79 | 0.63 |
| 2:B:33:C:H2' | 2:B:446:G:H22 | 1.64 | 0.63 |
| 2:B:1639:C:C2' | 2:B:1640:A:H5'' | 2.28 | 0.63 |
| 2:B:1197:G:H2' | 2:B:1198:U:H6 | 1.64 | 0.63 |
| 27:G:24:THR:HG22 | 27:G:34:ARG:HB3 | 1.81 | 0.63 |
| 2:B:141:G:C6 | 29:T:2:ILE:HG21 | 2.34 | 0.63 |
| 2:B:2809:A:H2' | 2:B:2810:A:C8 | 2.33 | 0.63 |
| 2:B:1796:U:H2' | 2:B:1797:G:C8 | 2.34 | 0.63 |
| 2:B:2813:A:H2' | 2:B:2814:A:C8 | 2.34 | 0.63 |
| 2:B:2100:G:H2' | 2:B:2101:A:C8 | 2.34 | 0.63 |
| 2:B:2595:G:H1 | 4:C:238:ASN:ND2 | 1.97 | 0.63 |
| 4:C:90:ILE:HD12 | 4:C:102:TYR:HB3 | 1.81 | 0.63 |
| 20:J:124:VAL:O | 20:J:125:TYR:HB2 | 1.97 | 0.63 |
| 2:B:2472:G:H2' | 2:B:2475:C:H42 | 1.63 | 0.63 |
| 7:P:88:ARG:HB2 | 7:P:112:ARG:NH1 | 2.13 | 0.63 |
| 19:H:31:VAL:CB | 19:H:32:PRO:CD | 2.75 | 0.63 |
| 7:P:56:SER:HB2 | 7:P:75:THR:CG2 | 2.28 | 0.63 |
| 26:F:102:LEU:HD13 | 26:F:103:ILE:HG13 | 1.80 | 0.63 |
| 26:F:62:GLN:HE22 | 26:F:90:LEU:HD13 | 1.64 | 0.63 |
| 2:B:721:A:H2' | 2:B:722:A:H8 | 1.64 | 0.63 |
| 29:T:50:LEU:H | 29:T:50:LEU:HD22 | 1.64 | 0.63 |
| 2:B:2579:C:O2' | 5:D:136:ASN:HA | 1.98 | 0.62 |
| 2:B:305:C:H2' | 2:B:306:U:C6 | 2.34 | 0.62 |
| 1:A:49:C:H2' | 1:A:50:A:C8 | 2.34 | 0.62 |
| 19:H:48:GLU:HA | 19:H:51:ARG:HE | 1.64 | 0.62 |
| 18:X:34:SER:HB2 | 18:X:36:GLN:OE1 | 1.98 | 0.62 |
| 23:Q:91:ARG:NH1 | 28:R:11:GLN:H | 1.97 | 0.62 |
| 2:B:543:G:C6 | 2:B:544:C:H1' | 2.33 | 0.62 |
| 19:H:133:GLN:HA | 19:H:138:VAL:O | 1.99 | 0.62 |
| 30:Z:66:THR:O | 30:Z:69:ALA:HB3 | 1.99 | 0.62 |
| 2:B:441:U:H2' | 2:B:442:G:H8 | 1.63 | 0.62 |
| 2:B:1060:U:O4 | 2:B:1088:A:N6 | 2.31 | 0.62 |
| 2:B:784:G:O2' | 2:B:785:G:H5'' | 2.00 | 0.62 |
| 2:B:191:A:H2' | 2:B:192:C:C6 | 2.34 | 0.62 |
| 2:B:1149:G:H2' | 2:B:1150:C:H6 | 1.64 | 0.62 |
| 2:B:1353:A:H2' | 2:B:1354:A:C8 | 2.33 | 0.62 |
| 2:B:155:A:H2' | 2:B:156:A:C8 | 2.34 | 0.62 |
| 2:B:1166:G:H2' | 2:B:1167:C:C6 | 2.34 | 0.62 |
| 4:C:129:LEU:HB3 | 4:C:134:ILE:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:Q:60:TRP:O | 23:Q:64:ILE:HG12 | 2.00 | 0.62 |
| 29:T:87:LEU:HD12 | 29:T:91:GLN:HG2 | 1.82 | 0.62 |
| 26:F:11:VAL:HG21 | 26:F:172:PHE:CE1 | 2.34 | 0.62 |
| 5:D:149:ASN:C | 5:D:152:PRO:HD2 | 2.20 | 0.62 |
| 2:B:1082:U:N3 | 2:B:1086:A:C6 | 2.67 | 0.62 |
| 25:U:10:VAL:O | 25:U:21:ARG:HA | 2.00 | 0.62 |
| 26:F:65:LEU:HD23 | 26:F:87:LYS:HD2 | 1.80 | 0.62 |
| 1:A:49:C:H2' | 1:A:50:A:H8 | 1.64 | 0.62 |
| 5:D:154:LYS:H | 5:D:154:LYS:HD3 | 1.63 | 0.62 |
| 31:W:18:LYS:HE3 | 31:W:36:ILE:HG12 | 1.81 | 0.62 |
| 31:W:49:ASN:HA | 31:W:61:LYS:H | 1.64 | 0.62 |
| 20:J:3:THR:HG21 | 23:Q:60:TRP:HE1 | 1.64 | 0.62 |
| 5:D:51:THR:HG21 | 5:D:76:GLY:HA3 | 1.82 | 0.62 |
| 3:I:20:SER:O | 3:I:25:PRO:HD2 | 1.99 | 0.62 |
| 27:G:115:GLN:H | 27:G:115:GLN:CD | 2.02 | 0.62 |
| 4:C:250:GLN:NE2 | 4:C:254:LYS:HE3 | 2.15 | 0.62 |
| 17:M:33:LEU:HD22 | 17:M:128:THR:HB | 1.80 | 0.62 |
| 2:B:458:G:N2 | 2:B:469:G:H2' | 2.15 | 0.62 |
| 2:B:1826:G:H2' | 2:B:1827:U:H6 | 1.64 | 0.62 |
| 16:L:93:ASN:H | 16:L:93:ASN:ND2 | 1.96 | 0.62 |
| 26:F:91:ARG:HD3 | 26:F:91:ARG:N | 2.14 | 0.62 |
| 4:C:75:ALA:HB1 | 4:C:93:VAL:HG22 | 1.80 | 0.62 |
| 2:B:1447:C:H2' | 2:B:1448:G:C8 | 2.32 | 0.62 |
| 2:B:1913:A:H4' | 2:B:1914:C:C5' | 2.29 | 0.62 |
| 4:C:166:ARG:HB3 | 4:C:171:VAL:HG22 | 1.81 | 0.62 |
| 2:B:90:U:H3' | 2:B:91:A:C5' | 2.27 | 0.62 |
| 2:B:163:C:H2' | 2:B:164:C:O4' | 1.99 | 0.62 |
| 2:B:594:U:H2' | 2:B:595:C:H6 | 1.62 | 0.62 |
| 1:A:74:U:H2' | 1:A:75:G:C8 | 2.34 | 0.62 |
| 2:B:2734:A:H2' | 2:B:2735:G:H5' | 1.82 | 0.62 |
| 2:B:1060:U:C5 | 3:I:131:THR:HG22 | 2.35 | 0.62 |
| 2:B:1553:A:O2' | 2:B:1554:U:H2' | 1.99 | 0.62 |
| 25:U:35:VAL:HB | 25:U:38:ILE:HB | 1.80 | 0.62 |
| 30:Z:39:TRP:HE1 | 30:Z:41:GLU:HG2 | 1.63 | 0.62 |
| 2:B:903:C:H2' | 2:B:904:G:H8 | 1.65 | 0.62 |
| 2:B:921:C:H2' | 2:B:922:C:H6 | 1.64 | 0.62 |
| 23:Q:83:LYS:NZ | 23:Q:87:VAL:HA | 2.15 | 0.62 |
| 27:G:102:ILE:HG13 | 27:G:116:LEU:HD11 | 1.81 | 0.62 |
| 2:B:2314:A:H4' | 26:F:34:THR:HG21 | 1.81 | 0.62 |
| 19:H:14:SER:HB3 | 19:H:17:ASP:CG | 2.20 | 0.62 |
| 1:A:32:U:C4' | 1:A:52:A:H62 | 2.12 | 0.62 |
| 19:H:65:ALA:CB | 19:H:138:VAL:HG21 | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:1387:A:H2' | 2:B:1388:G:C8 | 2.34 | 0.62 |
| 18:X:46:VAL:O | 18:X:50:VAL:HG23 | 2.00 | 0.62 |
| 2:B:2108:A:N3 | 2:B:2108:A:H2' | 2.14 | 0.62 |
| 2:B:115:C:O2' | 2:B:116:C:H5' | 1.99 | 0.62 |
| 5:D:39:ASP:HB3 | 5:D:42:ASN:HB3 | 1.80 | 0.62 |
| 2:B:402:A:H2' | 2:B:403:U:O4' | 2.00 | 0.62 |
| 8:E:5:LEU:HB2 | 8:E:10:SER:H | 1.63 | 0.62 |
| 6:K:105:ARG:HD3 | 6:K:105:ARG:H | 1.65 | 0.62 |
| 19:H:25:TYR:CD1 | 19:H:30:LEU:HG | 2.35 | 0.62 |
| 3:I:27:LEU:H | 3:I:27:LEU:CD2 | 2.12 | 0.62 |
| 25:U:78:LYS:HE3 | 25:U:79:ALA:N | 2.15 | 0.62 |
| 2:B:2814:A:H2' | 2:B:2815:C:C6 | 2.35 | 0.62 |
| 7:P:24:THR:O | 7:P:25:VAL:HG22 | 1.99 | 0.62 |
| 2:B:2267:A:N6 | 2:B:2272:U:C4 | 2.67 | 0.61 |
| 2:B:1177:G:H2' | 2:B:1178:C:C6 | 2.35 | 0.61 |
| 25:U:78:LYS:HD3 | 25:U:79:ALA:H | 1.64 | 0.61 |
| 6:K:119:ALA:HB3 | 6:K:120:PRO:HD3 | 1.82 | 0.61 |
| 6:K:13:ASN:HD21 | 6:K:98:ARG:H | 1.48 | 0.61 |
| 5:D:159:LYS:HA | 5:D:159:LYS:HZ3 | 1.63 | 0.61 |
| 7:P:56:SER:O | 7:P:75:THR:HG22 | 2.01 | 0.61 |
| 25:U:3:LYS:HB3 | 25:U:82:VAL:HG21 | 1.82 | 0.61 |
| 10:O:21:LEU:HD12 | 24:S:19:LEU:O | 2.00 | 0.61 |
| 2:B:1400:U:H2' | 2:B:1401:G:C8 | 2.34 | 0.61 |
| 2:B:2294:G:P | 22:O:94:ARG:HH11 | 2.23 | 0.61 |
| 2:B:921:C:H2' | 2:B:922:C:C6 | 2.36 | 0.61 |
| 19:H:147:VAL:HG12 | 19:H:148:ALA:H | 1.65 | 0.61 |
| 2:B:823:C:O2' | 2:B:824:U:H5' | 2.01 | 0.61 |
| 2:B:1733:G:H2' | 2:B:1734:G:C8 | 2.35 | 0.61 |
| 29:T:57:VAL:HG12 | 29:T:86:THR:OG1 | 2.01 | 0.61 |
| 26:F:32:LYS:HB2 | 26:F:90:LEU:O | 2.00 | 0.61 |
| 24:S:18:ARG:HB3 | 24:S:76:VAL:CG2 | 2.30 | 0.61 |
| 2:B:1716:U:H2' | 2:B:1717:A:C8 | 2.36 | 0.61 |
| 2:B:1015:U:H2' | 2:B:1016:G:H8 | 1.65 | 0.61 |
| 27:G:37:ASN:ND2 | 27:G:38:ASP:H | 1.97 | 0.61 |
| 31:W:23:LYS:HD2 | 31:W:24:ARG:N | 2.15 | 0.61 |
| 27:G:84:LYS:HB3 | 27:G:132:LEU:O | 2.01 | 0.61 |
| 25:U:51:LEU:H | 25:U:53:GLN:NE2 | 1.98 | 0.61 |
| 2:B:37:C:O2' | 8:E:45:ALA:HA | 2.01 | 0.61 |
| 2:B:702:U:H2' | 2:B:703:U:C6 | 2.36 | 0.61 |
| 27:G:23:ILE:HD11 | 27:G:42:VAL:HG11 | 1.83 | 0.61 |
| 7:P:58:PHE:CE2 | 7:P:75:THR:HB | 2.34 | 0.61 |
| 26:F:101:ARG:NH1 | 26:F:138:PRO:HB2 | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:F:90:LEU:C | 26:F:91:ARG:HD3 | 2.21 | 0.61 |
| 2:B:2675:A:H4' | 6:K:29:HIS:HB2 | 1.81 | 0.61 |
| 2:B:2728:U:H2' | 2:B:2729:G:C8 | 2.35 | 0.61 |
| 4:C:13:ARG:HG3 | 4:C:14:HIS:ND1 | 2.16 | 0.61 |
| 6:K:8:LEU:N | 6:K:8:LEU:HD12 | 2.15 | 0.61 |
| 2:B:1098:A:C8 | 3:I:3:LYS:HB3 | 2.36 | 0.61 |
| 2:B:2216:G:H2' | 2:B:2217:G:C8 | 2.35 | 0.61 |
| 20:J:6:ALA:HB3 | 20:J:45:THR:HG21 | 1.81 | 0.61 |
| 23:Q:104:ALA:HA | 28:R:46:GLU:OE2 | 2.01 | 0.61 |
| 29:T:32:LEU:N | 29:T:83:ALA:HB3 | 2.15 | 0.61 |
| 20:J:55:ILE:O | 20:J:55:ILE:HG13 | 2.01 | 0.61 |
| 4:C:16:VAL:H | 4:C:203:VAL:HG12 | 1.64 | 0.61 |
| 2:B:1196:C:H2' | 2:B:1197:G:C8 | 2.36 | 0.61 |
| 2:B:1585:C:H2' | 2:B:1586:A:O4' | 2.00 | 0.61 |
| 4:C:66:PHE:HB2 | 4:C:150:GLY:O | 2.00 | 0.61 |
| 2:B:1100:C:H2' | 2:B:1101:U:H6 | 1.65 | 0.61 |
| 27:G:36:LEU:HD22 | 27:G:36:LEU:H | 1.65 | 0.61 |
| 5:D:136:ASN:HD21 | 5:D:139:SER:C | 2.04 | 0.61 |
| 25:U:35:VAL:HB | 25:U:38:ILE:CB | 2.31 | 0.61 |
| 2:B:441:U:H2' | 2:B:442:G:C8 | 2.36 | 0.61 |
| 13:3:6:VAL:HB | 13:3:60:CYS:HB3 | 1.83 | 0.61 |
| 31:W:35:ILE:HG12 | 31:W:35:ILE:O | 2.00 | 0.61 |
| 30:Z:31:PRO:HB2 | 30:Z:33:LEU:CD1 | 2.31 | 0.61 |
| 5:D:148:GLN:HG3 | 5:D:152:PRO:CB | 2.30 | 0.61 |
| 2:B:1654:A:O2' | 5:D:118:PHE:HB2 | 2.00 | 0.61 |
| 2:B:639:U:H2' | 2:B:640:C:C6 | 2.36 | 0.61 |
| 20:J:30:THR:HG23 | 20:J:31:GLU:N | 2.16 | 0.61 |
| 24:S:81:SER:HA | 24:S:99:ARG:HA | 1.81 | 0.61 |
| 2:B:2105:U:H2' | 2:B:2106:U:O4' | 2.01 | 0.61 |
| 26:F:126:ASN:HD22 | 26:F:156:THR:HA | 1.66 | 0.60 |
| 27:G:86:LEU:HD22 | 27:G:161:VAL:HG12 | 1.82 | 0.60 |
| 12:1:26:LYS:HD2 | 12:1:30:PRO:HA | 1.81 | 0.60 |
| 10:0:41:HIS:HB3 | 21:N:99:LYS:HB2 | 1.82 | 0.60 |
| 2:B:171:U:H2' | 2:B:172:A:H8 | 1.64 | 0.60 |
| 13:3:22:LYS:HB2 | 13:3:48:MET:SD | 2.40 | 0.60 |
| 1:A:50:A:OP1 | 22:O:68:LYS:HG3 | 2.01 | 0.60 |
| 31:W:24:ARG:HD3 | 31:W:65:LYS:NZ | 2.16 | 0.60 |
| 19:H:32:PRO:O | 19:H:33:GLN:HB2 | 2.01 | 0.60 |
| 29:T:57:VAL:HG13 | 29:T:58:VAL:N | 2.16 | 0.60 |
| 31:W:37:VAL:HG13 | 31:W:55:ASP:O | 2.02 | 0.60 |
| 19:H:8:LYS:O | 19:H:13:GLY:HA3 | 2.01 | 0.60 |
| 2:B:1794:A:H2' | 2:B:1795:C:H6 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 18:X:52:ARG:O | 18:X:55:THR:HB | 2.01 | 0.60 |
| 2:B:2649:C:H2' | 2:B:2650:U:C6 | 2.36 | 0.60 |
| 14:V:21:ARG:HE | 14:V:87:GLN:HB3 | 1.66 | 0.60 |
| 14:V:80:HIS:HB3 | 14:V:83:LYS:O | 2.01 | 0.60 |
| 2:B:1400:U:H2' | 2:B:1401:G:H8 | 1.65 | 0.60 |
| 25:U:86:PHE:HB3 | 25:U:90:LYS:O | 2.00 | 0.60 |
| 27:G:36:LEU:HD22 | 27:G:36:LEU:N | 2.16 | 0.60 |
| 23:Q:83:LYS:HZ3 | 23:Q:87:VAL:HA | 1.66 | 0.60 |
| 2:B:1175:A:H2' | 2:B:1175:A:N3 | 2.14 | 0.60 |
| 21:N:101:GLY:HA2 | 21:N:110:MET:H | 1.66 | 0.60 |
| 17:M:57:VAL:HG13 | 17:M:108:VAL:HG21 | 1.83 | 0.60 |
| 2:B:233:A:N6 | 2:B:428:A:H61 | 1.98 | 0.60 |
| 4:C:181:ARG:HH22 | 4:C:265:PHE:HB3 | 1.66 | 0.60 |
| 2:B:2500:U:H5' | 2:B:2501:C:OP2 | 2.01 | 0.60 |
| 2:B:1098:A:C2' | 3:I:4:VAL:N | 2.64 | 0.60 |
| 14:V:31:TYR:HA | 14:V:93:ARG:NH2 | 2.17 | 0.60 |
| 16:L:79:LEU:HB2 | 16:L:113:ALA:H | 1.67 | 0.60 |
| 27:G:115:GLN:H | 27:G:115:GLN:NE2 | 1.99 | 0.60 |
| 1:A:2:G:H2' | 1:A:3:C:H6 | 1.65 | 0.60 |
| 2:B:1717:A:H2' | 2:B:1718:G:O4' | 2.02 | 0.60 |
| 2:B:1729:U:H3' | 2:B:1730:C:H4' | 1.82 | 0.60 |
| 2:B:659:G:H21 | 8:E:30:GLN:NE2 | 2.00 | 0.60 |
| 2:B:841:G:O2' | 2:B:842:U:H5' | 2.02 | 0.60 |
| 26:F:7:TYR:HA | 26:F:11:VAL:CG2 | 2.31 | 0.60 |
| 2:B:783:A:H2' | 2:B:784:G:O5' | 2.01 | 0.60 |
| 27:G:148:ARG:HA | 27:G:161:VAL:HB | 1.81 | 0.60 |
| 6:K:2:ILE:N | 6:K:2:ILE:HD12 | 2.16 | 0.60 |
| 28:R:7:SER:HB2 | 28:R:22:LEU:CB | 2.31 | 0.60 |
| 5:D:182:ALA:O | 5:D:184:ARG:HG2 | 2.00 | 0.60 |
| 11:4:7:VAL:HG13 | 11:4:8:LYS:N | 2.13 | 0.60 |
| 2:B:1439:A:H1' | 2:B:1553:A:N6 | 2.15 | 0.60 |
| 8:E:58:LYS:HE2 | 8:E:60:TRP:HD1 | 1.66 | 0.60 |
| 30:Z:76:GLU:HG3 | 30:Z:77:LYS:H | 1.67 | 0.60 |
| 25:U:11:ILE:HD13 | 25:U:20:LYS:H | 1.67 | 0.60 |
| 2:B:1870:C:H3' | 2:B:1871:A:H8 | 1.66 | 0.60 |
| 15:2:27:GLY:O | 15:2:30:VAL:HB | 2.02 | 0.60 |
| 2:B:1015:U:H2' | 2:B:1016:G:C8 | 2.37 | 0.60 |
| 8:E:108:ILE:HD13 | 8:E:108:ILE:O | 2.00 | 0.60 |
| 20:J:64:VAL:HG22 | 20:J:68:LYS:HD2 | 1.82 | 0.60 |
| 2:B:1464:G:H2' | 2:B:1465:G:H8 | 1.67 | 0.60 |
| 1:A:116:G:H4' | 22:O:54:VAL:HG22 | 1.83 | 0.60 |
| 3:I:32:VAL:HG22 | 3:I:60:VAL:HG21 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 9:Y:26:LEU:HD21 | 9:Y:46:MET:HB3 | 1.82 | 0.60 |
| 6:K:99:ILE:HG12 | 6:K:115:ILE:HG13 | 1.83 | 0.60 |
| 2:B:172:A:H2' | 2:B:173:A:H8 | 1.63 | 0.60 |
| 2:B:796:C:H2' | 2:B:797:G:C8 | 2.35 | 0.60 |
| 14:V:80:HIS:CD2 | 14:V:83:LYS:H | 2.20 | 0.60 |
| 2:B:1826:G:H2' | 2:B:1827:U:C6 | 2.37 | 0.60 |
| 4:C:54:GLY:O | 4:C:214:GLY:HA2 | 2.01 | 0.60 |
| 2:B:2772:C:H2' | 2:B:2773:C:H6 | 1.66 | 0.60 |
| 20:J:13:ARG:O | 20:J:52:ASP:HA | 2.02 | 0.60 |
| 20:J:103:ILE:HD12 | 20:J:104:ALA:N | 2.16 | 0.60 |
| 22:O:35:ILE:HD11 | 22:O:102:ARG:HE | 1.67 | 0.60 |
| 27:G:157:LYS:HB3 | 27:G:159:LYS:HG3 | 1.82 | 0.60 |
| 2:B:2081:U:OP1 | 30:Z:19:SER:HB3 | 2.01 | 0.60 |
| 2:B:813:U:H2' | 2:B:814:C:C6 | 2.37 | 0.60 |
| 28:R:6:GLN:HE22 | 28:R:10:LYS:N | 1.98 | 0.60 |
| 3:I:112:LYS:O | 3:I:116:MET:HG3 | 2.02 | 0.60 |
| 26:F:127:TYR:OH | 26:F:166:ARG:HG3 | 2.01 | 0.60 |
| 28:R:2:TYR:HB2 | 28:R:42:ALA:CB | 2.29 | 0.60 |
| 16:L:79:LEU:HB3 | 16:L:115:GLU:O | 2.01 | 0.60 |
| 19:H:133:GLN:HA | 19:H:139:PHE:HB3 | 1.84 | 0.60 |
| 2:B:2425:A:H5'' | 2:B:2426:A:H3' | 1.83 | 0.60 |
| 2:B:2358:A:H61 | 16:L:54:GLN:HE22 | 1.50 | 0.60 |
| 4:C:264:LYS:HG3 | 4:C:265:PHE:CD2 | 2.36 | 0.60 |
| 2:B:903:C:H2' | 2:B:904:G:C8 | 2.36 | 0.60 |
| 20:J:77:HIS:CD2 | 20:J:84:ILE:H | 2.20 | 0.60 |
| 7:P:99:LEU:HA | 7:P:102:ARG:HG3 | 1.82 | 0.60 |
| 2:B:2395:C:H2' | 2:B:2396:G:O4' | 2.01 | 0.60 |
| 2:B:2300:C:H2' | 2:B:2301:C:C6 | 2.37 | 0.60 |
| 31:W:39:GLN:HE21 | 31:W:42:THR:CB | 2.14 | 0.60 |
| 27:G:17:LYS:HB3 | 27:G:24:THR:H | 1.67 | 0.60 |
| 23:Q:63:ARG:CZ | 23:Q:96:ASP:HA | 2.32 | 0.60 |
| 24:S:31:GLN:O | 24:S:35:ILE:HG12 | 2.02 | 0.60 |
| 2:B:873:C:H4' | 17:M:64:TRP:HE1 | 1.67 | 0.60 |
| 2:B:1870:C:H3' | 2:B:1871:A:C8 | 2.36 | 0.60 |
| 2:B:479:A:N3 | 2:B:481:G:H5'' | 2.16 | 0.60 |
| 2:B:828:U:H4' | 2:B:831:G:N1 | 2.16 | 0.60 |
| 2:B:934:U:H2' | 2:B:935:C:C6 | 2.36 | 0.60 |
| 17:M:31:PHE:HD1 | 17:M:105:MET:HB3 | 1.66 | 0.60 |
| 2:B:1376:C:H3' | 35:B:3698:HOH:O | 2.02 | 0.60 |
| 2:B:1099:G:C8 | 3:I:3:LYS:HB2 | 2.37 | 0.59 |
| 2:B:854:C:O2' | 2:B:855:G:H5' | 2.01 | 0.59 |
| 16:L:143:GLU:CG | 16:L:144:GLU:H | 1.99 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 23:Q:63:ARG:HH12 | 23:Q:96:ASP:CB | 2.15 | 0.59 |
| 29:T:54:GLU:CB | 29:T:88:LYS:HB2 | 2.31 | 0.59 |
| 2:B:784:G:C6 | 4:C:227:VAL:HG11 | 2.37 | 0.59 |
| 2:B:138:U:H4' | 2:B:139:U:H2' | 1.84 | 0.59 |
| 2:B:19:A:H2' | 2:B:20:C:H6 | 1.66 | 0.59 |
| 2:B:898:C:O2 | 2:B:898:C:H2' | 2.02 | 0.59 |
| 2:B:1501:G:O2' | 2:B:1502:A:H5' | 2.01 | 0.59 |
| 31:W:48:ALA:O | 31:W:61:LYS:HB2 | 2.02 | 0.59 |
| 20:J:11:VAL:HG11 | 20:J:13:ARG:HE | 1.67 | 0.59 |
| 23:Q:73:ILE:HD11 | 23:Q:77:LYS:HB2 | 1.84 | 0.59 |
| 28:R:3:ALA:O | 28:R:13:ARG:HA | 2.02 | 0.59 |
| 28:R:4:VAL:HA | 28:R:12:HIS:O | 2.03 | 0.59 |
| 2:B:2746:U:H5'' | 27:G:137:LYS:HG2 | 1.82 | 0.59 |
| 31:W:37:VAL:HG12 | 31:W:38:ARG:HD3 | 1.83 | 0.59 |
| 2:B:528:A:N1 | 2:B:2042:A:H2' | 2.17 | 0.59 |
| 2:B:1335:C:H2' | 2:B:1336:A:C8 | 2.37 | 0.59 |
| 2:B:1794:A:H2' | 2:B:1795:C:C6 | 2.36 | 0.59 |
| 2:B:254:G:N2 | 13:3:7:ARG:HH21 | 2.00 | 0.59 |
| 2:B:102:U:C6 | 18:X:2:LYS:HE3 | 2.37 | 0.59 |
| 23:Q:9:ALA:C | 23:Q:11:ALA:H | 2.04 | 0.59 |
| 2:B:1722:A:H2' | 2:B:1723:G:C8 | 2.37 | 0.59 |
| 2:B:184:C:H2' | 2:B:185:G:H8 | 1.67 | 0.59 |
| 2:B:2366:A:H2' | 2:B:2367:G:O4' | 2.02 | 0.59 |
| 16:L:121:THR:HG22 | 16:L:141:LYS:HB3 | 1.83 | 0.59 |
| 4:C:138:SER:O | 4:C:140:VAL:HG23 | 2.02 | 0.59 |
| 25:U:85:ARG:HH11 | 25:U:86:PHE:H | 1.49 | 0.59 |
| 2:B:1812:U:C1' | 4:C:43:ASN:HD21 | 2.11 | 0.59 |
| 14:V:72:VAL:HB | 14:V:92:VAL:O | 2.02 | 0.59 |
| 2:B:30:G:H2' | 2:B:31:C:H6 | 1.68 | 0.59 |
| 29:T:29:THR:HB | 29:T:86:THR:HG22 | 1.84 | 0.59 |
| 9:Y:15:ARG:O | 9:Y:20:LYS:HE3 | 2.01 | 0.59 |
| 2:B:2144:G:H2' | 2:B:2145:C:O3' | 2.03 | 0.59 |
| 2:B:2148:G:H3' | 2:B:2148:G:OP2 | 2.03 | 0.59 |
| 2:B:2834:G:H1' | 2:B:2883:A:N6 | 2.18 | 0.59 |
| 2:B:2393:U:H5'' | 16:L:62:PRO:HG3 | 1.84 | 0.59 |
| 2:B:2229:U:H2' | 2:B:2230:G:C8 | 2.37 | 0.59 |
| 20:J:59:ALA:O | 20:J:62:VAL:HG12 | 2.01 | 0.59 |
| 2:B:265:A:O2' | 2:B:266:G:H4' | 2.02 | 0.59 |
| 25:U:23:LYS:HD2 | 25:U:23:LYS:H | 1.67 | 0.59 |
| 2:B:2331:G:H4' | 31:W:39:GLN:HA | 1.83 | 0.59 |
| 27:G:9:VAL:HG12 | 27:G:11:PRO:HD3 | 1.83 | 0.59 |
| 29:T:38:ALA:O | 29:T:39:THR:HB | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 26:F:11:VAL:HG21 | 26:F:172:PHE:HE1 | 1.66 | 0.59 |
| 19:H:21:VAL:HG11 | 19:H:30:LEU:HD12 | 1.84 | 0.59 |
| 2:B:608:A:H2' | 2:B:609:A:C8 | 2.36 | 0.59 |
| 22:O:74:VAL:O | 22:O:78:VAL:HG22 | 2.02 | 0.59 |
| 2:B:2841:C:H2' | 2:B:2842:G:H8 | 1.68 | 0.59 |
| 7:P:62:LYS:HE3 | 7:P:64:SER:OG | 2.01 | 0.59 |
| 2:B:2150:C:H2' | 2:B:2151:U:H6 | 1.66 | 0.59 |
| 2:B:2860:A:O5' | 2:B:2860:A:H8 | 1.85 | 0.59 |
| 25:U:23:LYS:HD2 | 25:U:23:LYS:N | 2.18 | 0.59 |
| 2:B:1739:A:H2' | 2:B:1740:G:O4' | 2.01 | 0.59 |
| 16:L:89:VAL:HG23 | 16:L:123:ARG:HB2 | 1.85 | 0.59 |
| 26:F:163:GLU:HA | 26:F:166:ARG:HH11 | 1.66 | 0.59 |
| 7:P:52:ARG:HG2 | 7:P:52:ARG:HH11 | 1.68 | 0.59 |
| 2:B:277:G:H4' | 2:B:278:A:N7 | 2.17 | 0.59 |
| 25:U:82:VAL:HG13 | 25:U:93:ARG:HB3 | 1.84 | 0.59 |
| 21:N:45:ARG:HG3 | 21:N:95:THR:HG21 | 1.85 | 0.59 |
| 4:C:158:GLY:N | 4:C:194:VAL:HG13 | 2.18 | 0.59 |
| 18:X:29:ARG:HH12 | 29:T:12:ARG:HA | 1.68 | 0.59 |
| 19:H:64:ALA:O | 19:H:68:ARG:HG2 | 2.02 | 0.59 |
| 2:B:1745:A:H2' | 2:B:1746:A:O4' | 2.02 | 0.59 |
| 5:D:8:LYS:HB2 | 5:D:201:LEU:HD21 | 1.83 | 0.59 |
| 2:B:2530:A:H5' | 27:G:174:LYS:HD2 | 1.85 | 0.59 |
| 21:N:49:GLU:OE2 | 21:N:95:THR:HG22 | 2.03 | 0.59 |
| 8:E:46:GLN:HG3 | 8:E:87:ALA:HB3 | 1.83 | 0.59 |
| 4:C:239:PHE:O | 4:C:241:LYS:HG3 | 2.03 | 0.59 |
| 2:B:720:U:H2' | 2:B:721:A:H8 | 1.65 | 0.59 |
| 2:B:2065:C:H2' | 2:B:2066:C:H6 | 1.68 | 0.59 |
| 8:E:150:THR:HG21 | 8:E:153:LEU:HA | 1.83 | 0.59 |
| 2:B:208:C:H2' | 2:B:209:C:C6 | 2.37 | 0.59 |
| 2:B:1117:C:O2' | 2:B:1118:C:H5' | 2.02 | 0.59 |
| 2:B:674:G:H4' | 8:E:69:ARG:HB3 | 1.85 | 0.59 |
| 2:B:1771:C:O2' | 2:B:1772:A:H5' | 2.02 | 0.59 |
| 2:B:2186:G:H2' | 2:B:2187:U:O4' | 2.03 | 0.59 |
| 22:O:6:ALA:O | 22:O:10:ARG:HG3 | 2.02 | 0.59 |
| 2:B:2354:C:H4' | 31:W:31:LEU:HD23 | 1.84 | 0.59 |
| 4:C:143:VAL:HG12 | 4:C:144:GLU:N | 2.17 | 0.59 |
| 2:B:1812:U:H2' | 2:B:1813:G:H8 | 1.68 | 0.59 |
| 2:B:704:G:C2' | 2:B:726:G:H22 | 2.10 | 0.59 |
| 29:T:25:GLU:HA | 29:T:28:ASN:O | 2.02 | 0.59 |
| 26:F:155:ILE:HG21 | 26:F:169:LEU:HD21 | 1.84 | 0.59 |
| 20:J:93:ILE:O | 20:J:97:PRO:HG3 | 2.02 | 0.59 |
| 30:Z:27:ARG:HD3 | 30:Z:28:ARG:N | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 22:O:6:ALA:HB3 | 22:O:10:ARG:HH11 | 1.67 | 0.59 |
| 2:B:2400:G:O2' | 2:B:2401:U:H5' | 2.02 | 0.59 |
| 1:A:10:G:H2' | 1:A:11:C:O4' | 2.03 | 0.59 |
| 25:U:26:ASN:HB3 | 25:U:34:ILE:HD12 | 1.85 | 0.59 |
| 24:S:25:ARG:HE | 24:S:74:ILE:HG23 | 1.67 | 0.59 |
| 2:B:2571:U:O2' | 5:D:152:PRO:HG3 | 2.03 | 0.59 |
| 6:K:54:LYS:N | 6:K:54:LYS:HD2 | 2.16 | 0.59 |
| 8:E:188:MET:HG2 | 8:E:193:VAL:CG2 | 2.32 | 0.59 |
| 2:B:1827:U:C2' | 2:B:1828:G:H5' | 2.32 | 0.59 |
| 2:B:2216:G:H2' | 2:B:2217:G:H8 | 1.65 | 0.59 |
| 2:B:235:U:H2' | 2:B:236:C:C6 | 2.38 | 0.59 |
| 1:A:59:A:H2' | 1:A:60:C:O4' | 2.03 | 0.59 |
| 7:P:75:THR:HG23 | 7:P:76:HIS:N | 2.16 | 0.59 |
| 3:I:78:LEU:HA | 3:I:81:LYS:HE2 | 1.84 | 0.59 |
| 2:B:2386:A:C2 | 31:W:38:ARG:HB3 | 2.38 | 0.59 |
| 2:B:1820:U:OP1 | 4:C:176:ARG:HD2 | 2.03 | 0.59 |
| 8:E:195:GLN:O | 8:E:198:GLU:HG2 | 2.03 | 0.59 |
| 2:B:1661:G:O2' | 2:B:1662:U:H5' | 2.02 | 0.59 |
| 2:B:1923:U:H2' | 2:B:1924:C:C6 | 2.38 | 0.59 |
| 29:T:43:ILE:O | 29:T:47:VAL:HG23 | 2.03 | 0.58 |
| 10:O:28:SER:HB2 | 10:O:39:ARG:HG2 | 1.84 | 0.58 |
| 20:J:17:VAL:HG22 | 20:J:55:ILE:HD11 | 1.85 | 0.58 |
| 2:B:1082:U:C2 | 2:B:1086:A:C6 | 2.90 | 0.58 |
| 25:U:35:VAL:HB | 25:U:38:ILE:CG2 | 2.33 | 0.58 |
| 6:K:64:ARG:HD2 | 6:K:102:PRO:O | 2.02 | 0.58 |
| 6:K:120:PRO:HA | 7:P:65:ASN:ND2 | 2.17 | 0.58 |
| 2:B:62:U:H3' | 2:B:63:A:H8 | 1.66 | 0.58 |
| 2:B:634:C:H2' | 2:B:635:C:C6 | 2.37 | 0.58 |
| 2:B:2106:U:H2' | 2:B:2107:G:H8 | 1.67 | 0.58 |
| 20:J:11:VAL:HG11 | 20:J:13:ARG:NE | 2.17 | 0.58 |
| 27:G:140:ILE:HD12 | 27:G:141:GLY:N | 2.18 | 0.58 |
| 23:Q:78:PHE:CZ | 23:Q:82:LEU:HD11 | 2.39 | 0.58 |
| 8:E:46:GLN:HB3 | 8:E:86:ALA:HA | 1.85 | 0.58 |
| 18:X:48:ARG:O | 18:X:51:ALA:HB3 | 2.02 | 0.58 |
| 28:R:60:LYS:N | 28:R:100:GLY:HA3 | 2.08 | 0.58 |
| 29:T:32:LEU:H | 29:T:83:ALA:HB3 | 1.69 | 0.58 |
| 29:T:39:THR:CG2 | 29:T:42:GLU:H | 2.16 | 0.58 |
| 26:F:16:MET:O | 26:F:20:ASN:HA | 2.02 | 0.58 |
| 21:N:24:MET:HE2 | 21:N:44:LEU:HB2 | 1.83 | 0.58 |
| 2:B:2849:U:H4' | 2:B:2850:A:C5' | 2.33 | 0.58 |
| 2:B:654:A:C2' | 2:B:655:A:H5'' | 2.33 | 0.58 |
| 2:B:2346:A:H3' | 2:B:2347:C:H5'' | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:1419:A:H2' | 2:B:1421:G:N7 | 2.17 | 0.58 |
| 15:2:3:ARG:HA | 15:2:3:ARG:NE | 2.18 | 0.58 |
| 16:L:110:VAL:HG23 | 16:L:126:ARG:O | 2.03 | 0.58 |
| 19:H:62:LEU:CG | 19:H:66:ASN:HD21 | 2.11 | 0.58 |
| 17:M:40:ARG:HB2 | 17:M:93:VAL:HG21 | 1.86 | 0.58 |
| 2:B:2484:G:OP1 | 17:M:44:ARG:HD3 | 2.02 | 0.58 |
| 26:F:107:VAL:O | 26:F:110:ILE:HG22 | 2.04 | 0.58 |
| 20:J:18:VAL:HG12 | 20:J:54:ILE:HD11 | 1.85 | 0.58 |
| 4:C:77:VAL:HG23 | 4:C:112:GLY:N | 2.19 | 0.58 |
| 15:2:3:ARG:HA | 15:2:3:ARG:CZ | 2.33 | 0.58 |
| 20:J:23:LYS:NZ | 20:J:142:ILE:HG12 | 2.19 | 0.58 |
| 24:S:72:THR:HG21 | 24:S:108:SER:HB3 | 1.84 | 0.58 |
| 31:W:59:PHE:CD2 | 31:W:61:LYS:HD2 | 2.39 | 0.58 |
| 19:H:82:SER:OG | 19:H:94:ILE:HD13 | 2.03 | 0.58 |
| 2:B:1181:U:H2' | 2:B:1182:G:H8 | 1.67 | 0.58 |
| 27:G:85:LYS:HB2 | 27:G:164:ALA:HB3 | 1.86 | 0.58 |
| 2:B:2571:U:H4' | 5:D:151:THR:HG21 | 1.84 | 0.58 |
| 2:B:1082:U:O4 | 2:B:1086:A:C2 | 2.56 | 0.58 |
| 3:I:125:THR:O | 3:I:129:GLU:HG3 | 2.04 | 0.58 |
| 2:B:192:C:C2' | 2:B:193:U:H5' | 2.33 | 0.58 |
| 2:B:825:A:H1' | 16:L:54:GLN:HE21 | 1.68 | 0.58 |
| 2:B:946:C:H2' | 2:B:947:A:H8 | 1.68 | 0.58 |
| 2:B:1722:A:H2' | 2:B:1723:G:H8 | 1.69 | 0.58 |
| 2:B:2340:A:H2' | 2:B:2341:G:H8 | 1.67 | 0.58 |
| 2:B:2438:U:O2' | 2:B:2439:A:H5'' | 2.03 | 0.58 |
| 2:B:2026:U:H2' | 2:B:2027:G:H8 | 1.68 | 0.58 |
| 31:W:39:GLN:NE2 | 31:W:42:THR:HB | 2.13 | 0.58 |
| 28:R:66:HIS:ND1 | 28:R:94:THR:HG22 | 2.18 | 0.58 |
| 29:T:32:LEU:HG | 29:T:83:ALA:HB2 | 1.86 | 0.58 |
| 2:B:139:U:N3 | 29:T:1:MET:HB3 | 2.18 | 0.58 |
| 19:H:132:PHE:HD2 | 19:H:134:VAL:HG22 | 1.69 | 0.58 |
| 8:E:119:ILE:HD11 | 8:E:185:LYS:NZ | 2.19 | 0.58 |
| 2:B:1198:U:H2' | 2:B:1199:U:C6 | 2.38 | 0.58 |
| 2:B:2841:C:H2' | 2:B:2842:G:C8 | 2.38 | 0.58 |
| 2:B:1783:A:H5' | 2:B:2608:G:H4' | 1.85 | 0.58 |
| 2:B:794:A:H2' | 2:B:795:C:C6 | 2.37 | 0.58 |
| 24:S:55:ILE:O | 24:S:58:ALA:HB3 | 2.04 | 0.58 |
| 30:Z:59:ILE:HG22 | 30:Z:64:ILE:HG13 | 1.85 | 0.58 |
| 20:J:136:GLN:N | 20:J:137:PRO:HD3 | 2.19 | 0.58 |
| 25:U:9:GLU:OE2 | 25:U:21:ARG:HD2 | 2.04 | 0.58 |
| 2:B:2804:U:H2' | 2:B:2805:C:H6 | 1.67 | 0.58 |
| 2:B:233:A:H61 | 2:B:428:A:H61 | 1.48 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:417:C:H2' | 2:B:418:C:H6 | 1.69 | 0.58 |
| 2:B:2240:U:O2' | 2:B:2241:A:H5' | 2.04 | 0.58 |
| 2:B:321:U:OP2 | 8:E:130:LYS:HD3 | 2.04 | 0.58 |
| 2:B:1099:G:C8 | 3:I:3:LYS:CA | 2.82 | 0.58 |
| 31:W:18:LYS:HG3 | 31:W:19:ARG:CZ | 2.34 | 0.58 |
| 2:B:2052:A:O4' | 5:D:147:GLY:HA3 | 2.03 | 0.58 |
| 12:1:33:LEU:HB3 | 12:1:51:ALA:CB | 2.33 | 0.58 |
| 2:B:2728:U:H2' | 2:B:2729:G:H8 | 1.69 | 0.58 |
| 2:B:1405:U:H2' | 2:B:1406:U:C6 | 2.39 | 0.58 |
| 2:B:2085:U:O2' | 2:B:2086:U:H5' | 2.04 | 0.58 |
| 2:B:2229:U:H2' | 2:B:2230:G:H8 | 1.67 | 0.58 |
| 2:B:264:C:O2' | 2:B:265:A:H5'' | 2.04 | 0.58 |
| 2:B:1866:A:H2' | 2:B:1867:G:O4' | 2.04 | 0.58 |
| 2:B:1098:A:OP2 | 3:I:3:LYS:HG2 | 2.03 | 0.58 |
| 18:X:39:GLN:O | 18:X:42:LEU:HB2 | 2.04 | 0.58 |
| 20:J:44:TYR:O | 20:J:45:THR:HB | 2.03 | 0.58 |
| 4:C:171:VAL:HB | 4:C:183:VAL:HG12 | 1.86 | 0.58 |
| 24:S:18:ARG:HB3 | 24:S:76:VAL:HG22 | 1.86 | 0.58 |
| 23:Q:75:TYR:O | 23:Q:79:ILE:HG22 | 2.04 | 0.58 |
| 2:B:1018:U:O2' | 2:B:1019:U:H5' | 2.03 | 0.58 |
| 2:B:1551:A:H3' | 2:B:1552:A:H5'' | 1.84 | 0.58 |
| 2:B:170:U:H2' | 2:B:171:U:C6 | 2.39 | 0.58 |
| 4:C:181:ARG:NH2 | 4:C:265:PHE:HB3 | 2.18 | 0.58 |
| 2:B:899:A:C2 | 2:B:900:A:H1' | 2.39 | 0.58 |
| 29:T:49:LYS:HB2 | 29:T:50:LEU:HD22 | 1.86 | 0.58 |
| 2:B:2153:C:H2' | 2:B:2154:A:H8 | 1.69 | 0.58 |
| 2:B:2700:A:H2' | 2:B:2701:U:C6 | 2.39 | 0.58 |
| 1:A:24:G:O2' | 1:A:25:U:H5'' | 2.04 | 0.58 |
| 2:B:431:U:O2' | 2:B:432:A:H5' | 2.04 | 0.58 |
| 4:C:32:LEU:O | 4:C:63:ILE:HG12 | 2.03 | 0.58 |
| 14:V:4:ILE:HB | 14:V:63:ILE:HA | 1.85 | 0.58 |
| 24:S:33:LEU:HG | 24:S:51:LEU:HD23 | 1.85 | 0.58 |
| 27:G:174:LYS:NZ | 27:G:176:LYS:HG2 | 2.18 | 0.58 |
| 18:X:3:ALA:O | 18:X:6:LEU:HB2 | 2.04 | 0.58 |
| 2:B:968:C:H2' | 2:B:969:G:H8 | 1.67 | 0.58 |
| 2:B:2153:C:H2' | 2:B:2154:A:C8 | 2.38 | 0.58 |
| 1:A:90:C:OP1 | 17:M:16:ARG:HB2 | 2.04 | 0.58 |
| 23:Q:103:VAL:O | 23:Q:106:THR:HB | 2.03 | 0.58 |
| 23:Q:94:LEU:CD1 | 28:R:13:ARG:HB2 | 2.34 | 0.57 |
| 3:I:108:ILE:HG22 | 3:I:128:ILE:HD13 | 1.86 | 0.57 |
| 2:B:2886:A:N7 | 10:0:39:ARG:NH2 | 2.49 | 0.57 |
| 2:B:1548:A:H2' | 2:B:1549:A:C8 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:I:121:ILE:CD1 | 3:I:121:ILE:H | 2.14 | 0.57 |
| 29:T:18:GLU:C | 29:T:20:ALA:H | 2.07 | 0.57 |
| 2:B:173:A:H2' | 2:B:174:U:C6 | 2.39 | 0.57 |
| 2:B:1484:U:H2' | 2:B:1485:U:H6 | 1.69 | 0.57 |
| 15:2:30:VAL:HA | 15:2:33:ARG:NH2 | 2.19 | 0.57 |
| 18:X:51:ALA:O | 18:X:55:THR:N | 2.37 | 0.57 |
| 2:B:2086:U:H2' | 2:B:2087:G:C8 | 2.38 | 0.57 |
| 2:B:2840:C:H2' | 2:B:2841:C:H6 | 1.69 | 0.57 |
| 1:A:60:C:H2' | 1:A:61:G:H8 | 1.69 | 0.57 |
| 21:N:71:ARG:HH21 | 21:N:71:ARG:HG2 | 1.68 | 0.57 |
| 18:X:59:GLU:N | 18:X:59:GLU:CD | 2.57 | 0.57 |
| 2:B:956:G:N2 | 2:B:959:A:H3' | 2.19 | 0.57 |
| 4:C:229:HIS:ND1 | 4:C:230:PRO:HD2 | 2.19 | 0.57 |
| 21:N:17:ARG:C | 21:N:19:ALA:H | 2.06 | 0.57 |
| 16:L:125:LEU:H | 16:L:143:GLU:HG3 | 1.70 | 0.57 |
| 2:B:1180:U:H2' | 2:B:1181:U:C6 | 2.39 | 0.57 |
| 26:F:102:LEU:HD22 | 26:F:103:ILE:N | 2.19 | 0.57 |
| 26:F:109:ARG:HB3 | 26:F:135:ILE:HD12 | 1.85 | 0.57 |
| 26:F:169:LEU:O | 26:F:174:PHE:HB2 | 2.05 | 0.57 |
| 2:B:2720:U:H5'' | 7:P:52:ARG:HH22 | 1.68 | 0.57 |
| 17:M:100:LYS:HD3 | 17:M:101:VAL:H | 1.67 | 0.57 |
| 2:B:1230:A:H2' | 2:B:1231:U:H6 | 1.68 | 0.57 |
| 2:B:152:A:H2' | 2:B:153:U:C6 | 2.39 | 0.57 |
| 2:B:1132:U:H6 | 2:B:1132:U:H5' | 1.69 | 0.57 |
| 2:B:962:G:N2 | 2:B:2250:G:H1 | 2.02 | 0.57 |
| 13:3:41:ARG:HG3 | 13:3:44:ARG:HH22 | 1.69 | 0.57 |
| 2:B:1528:A:H2' | 2:B:1529:G:O4' | 2.03 | 0.57 |
| 31:W:23:LYS:HZ2 | 31:W:24:ARG:HG3 | 1.68 | 0.57 |
| 27:G:17:LYS:O | 27:G:23:ILE:HG23 | 2.03 | 0.57 |
| 23:Q:63:ARG:HH12 | 23:Q:96:ASP:CA | 2.16 | 0.57 |
| 27:G:84:LYS:HG2 | 27:G:85:LYS:N | 2.16 | 0.57 |
| 1:A:7:G:H1' | 22:O:38:GLN:HE22 | 1.68 | 0.57 |
| 2:B:1085:A:H1' | 2:B:1105:U:H1' | 1.85 | 0.57 |
| 17:M:108:VAL:HG22 | 17:M:109:PRO:HD2 | 1.86 | 0.57 |
| 2:B:2861:U:H2' | 2:B:2862:G:C8 | 2.40 | 0.57 |
| 2:B:2814:A:H2' | 2:B:2815:C:H6 | 1.68 | 0.57 |
| 2:B:2595:G:H1 | 4:C:238:ASN:HD21 | 1.53 | 0.57 |
| 2:B:958:U:H3 | 17:M:16:ARG:HB3 | 1.69 | 0.57 |
| 28:R:54:VAL:HG22 | 28:R:56:GLY:H | 1.68 | 0.57 |
| 2:B:1441:G:H2' | 2:B:1442:U:C6 | 2.39 | 0.57 |
| 2:B:278:A:H61 | 2:B:362:A:N6 | 2.02 | 0.57 |
| 12:1:29:LYS:N | 12:1:30:PRO:HD3 | 2.19 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2722:G:H2' | 2:B:2723:C:C6 | 2.39 | 0.57 |
| 12:1:36:LYS:HG2 | 12:1:47:ILE:HA | 1.86 | 0.57 |
| 2:B:2772:C:H2' | 2:B:2773:C:C6 | 2.39 | 0.57 |
| 2:B:5:A:H2' | 2:B:6:A:C8 | 2.39 | 0.57 |
| 2:B:1316:U:O2' | 2:B:1317:G:H5' | 2.03 | 0.57 |
| 2:B:871:U:H2' | 2:B:872:U:H6 | 1.69 | 0.57 |
| 2:B:1577:C:H2' | 2:B:1578:U:C6 | 2.39 | 0.57 |
| 2:B:2292:U:H2' | 2:B:2293:G:H8 | 1.69 | 0.57 |
| 2:B:554:U:H2' | 2:B:555:G:O4' | 2.04 | 0.57 |
| 23:Q:77:LYS:HA | 23:Q:80:ASN:HB3 | 1.87 | 0.57 |
| 25:U:35:VAL:HB | 25:U:38:ILE:HG21 | 1.87 | 0.57 |
| 2:B:718:A:H2' | 2:B:719:C:H5' | 1.85 | 0.57 |
| 2:B:2602:A:H3' | 2:B:2602:A:OP1 | 2.05 | 0.57 |
| 2:B:322:A:H5' | 2:B:340:A:H1' | 1.86 | 0.57 |
| 2:B:1877:A:H2' | 2:B:1878:G:C8 | 2.39 | 0.57 |
| 30:Z:70:GLU:O | 30:Z:72:ARG:N | 2.37 | 0.57 |
| 20:J:45:THR:HG23 | 20:J:45:THR:O | 2.04 | 0.57 |
| 28:R:49:ILE:HD13 | 28:R:51:VAL:O | 2.05 | 0.57 |
| 21:N:29:VAL:HG13 | 21:N:83:LEU:HD21 | 1.87 | 0.57 |
| 17:M:40:ARG:HB3 | 17:M:95:LEU:HD12 | 1.87 | 0.57 |
| 30:Z:3:ARG:HA | 30:Z:50:ARG:NH1 | 2.20 | 0.57 |
| 16:L:4:ASN:N | 16:L:4:ASN:HD22 | 2.02 | 0.57 |
| 2:B:277:G:N3 | 2:B:277:G:H2' | 2.19 | 0.57 |
| 2:B:1139:G:O2' | 2:B:1140:C:H5' | 2.03 | 0.57 |
| 7:P:91:VAL:O | 7:P:92:ARG:HB3 | 2.04 | 0.57 |
| 21:N:98:LEU:O | 21:N:112:TYR:HB2 | 2.04 | 0.57 |
| 2:B:1517:G:O2' | 2:B:1518:C:H5' | 2.04 | 0.57 |
| 2:B:1827:U:O2' | 2:B:1828:G:H5' | 2.05 | 0.57 |
| 22:O:6:ALA:O | 22:O:9:ARG:HG3 | 2.03 | 0.57 |
| 1:A:94:A:H2' | 1:A:95:U:O4' | 2.04 | 0.57 |
| 2:B:106:C:H2' | 2:B:107:G:H8 | 1.68 | 0.57 |
| 2:B:1241:A:H2' | 2:B:1242:U:H5' | 1.86 | 0.57 |
| 3:I:99:LYS:H | 3:I:99:LYS:HD3 | 1.69 | 0.57 |
| 4:C:226:PRO:HA | 4:C:232:GLY:HA3 | 1.85 | 0.57 |
| 25:U:27:VAL:HG23 | 25:U:33:VAL:HG12 | 1.86 | 0.57 |
| 31:W:18:LYS:HA | 31:W:36:ILE:HG12 | 1.87 | 0.57 |
| 16:L:108:ALA:HB3 | 16:L:125:LEU:HD21 | 1.87 | 0.57 |
| 21:N:72:ASP:HB3 | 21:N:75:ILE:CG1 | 2.35 | 0.57 |
| 2:B:360:U:H2' | 2:B:361:G:C8 | 2.40 | 0.57 |
| 2:B:1055:G:HO2' | 2:B:1085:A:H2 | 1.53 | 0.57 |
| 2:B:2732:G:H3' | 2:B:2733:A:H5' | 1.85 | 0.57 |
| 28:R:61:ALA:HB2 | 28:R:98:ILE:HA | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:E:181:ILE:HG13 | 16:L:2:ARG:HB3 | 1.86 | 0.57 |
| 2:B:438:G:H2' | 2:B:439:A:H8 | 1.70 | 0.57 |
| 2:B:833:A:H2' | 2:B:834:G:C8 | 2.40 | 0.57 |
| 2:B:699:A:H2' | 2:B:700:G:O4' | 2.04 | 0.57 |
| 2:B:1373:A:H2' | 2:B:1374:G:O4' | 2.05 | 0.57 |
| 31:W:59:PHE:O | 31:W:60:ALA:HB3 | 2.05 | 0.57 |
| 23:Q:77:LYS:O | 23:Q:80:ASN:HB3 | 2.04 | 0.57 |
| 5:D:109:VAL:HG11 | 5:D:193:VAL:HB | 1.87 | 0.57 |
| 4:C:102:TYR:O | 4:C:103:ILE:HG13 | 2.05 | 0.57 |
| 2:B:1168:G:H2' | 2:B:1169:A:H8 | 1.64 | 0.57 |
| 2:B:2646:C:H2' | 2:B:2647:U:O4' | 2.04 | 0.57 |
| 19:H:72:ILE:HG22 | 19:H:142:VAL:HG21 | 1.86 | 0.57 |
| 25:U:80:ASP:OD1 | 25:U:95:PHE:HB3 | 2.05 | 0.57 |
| 8:E:48:THR:HG22 | 8:E:86:ALA:HB3 | 1.87 | 0.57 |
| 2:B:1470:A:H3' | 2:B:1471:G:H8 | 1.68 | 0.57 |
| 2:B:1676:A:H2' | 2:B:1677:A:O4' | 2.05 | 0.57 |
| 2:B:1494:A:H2' | 2:B:1495:A:C8 | 2.39 | 0.57 |
| 2:B:324:A:H2' | 2:B:325:G:O4' | 2.04 | 0.57 |
| 27:G:49:LEU:HD12 | 27:G:49:LEU:N | 2.20 | 0.57 |
| 29:T:69:ARG:NE | 29:T:69:ARG:HA | 2.20 | 0.57 |
| 2:B:1203:U:H3' | 2:B:1204:A:H5'' | 1.85 | 0.57 |
| 2:B:141:G:O6 | 29:T:2:ILE:HD12 | 2.04 | 0.57 |
| 7:P:59:THR:OG1 | 7:P:72:VAL:HG12 | 2.05 | 0.57 |
| 26:F:147:ARG:HD2 | 26:F:148:VAL:HG22 | 1.85 | 0.57 |
| 2:B:2899:A:H2' | 2:B:2900:A:C8 | 2.40 | 0.57 |
| 4:C:4:LYS:HE2 | 4:C:5:CYS:H | 1.68 | 0.57 |
| 21:N:73:ASN:O | 21:N:76:VAL:HG22 | 2.05 | 0.57 |
| 19:H:12:LEU:HD11 | 19:H:30:LEU:HD11 | 1.87 | 0.57 |
| 2:B:143:C:H2' | 2:B:144:A:C8 | 2.40 | 0.57 |
| 29:T:2:ILE:HD13 | 29:T:2:ILE:N | 2.20 | 0.57 |
| 17:M:36:VAL:HB | 17:M:127:LYS:O | 2.04 | 0.57 |
| 18:X:53:VAL:O | 18:X:57:LEU:HD23 | 2.05 | 0.57 |
| 26:F:42:ALA:O | 26:F:46:LYS:HG3 | 2.04 | 0.57 |
| 2:B:2078:C:O2' | 2:B:2079:U:H5' | 2.05 | 0.57 |
| 2:B:969:G:H2' | 2:B:970:U:C6 | 2.39 | 0.57 |
| 2:B:962:G:H21 | 2:B:2250:G:H1 | 1.53 | 0.57 |
| 2:B:300:A:H2' | 2:B:334:C:H1' | 1.87 | 0.57 |
| 2:B:1878:G:H2' | 2:B:1879:C:C6 | 2.39 | 0.57 |
| 2:B:1028:A:H2' | 2:B:1029:A:C8 | 2.40 | 0.57 |
| 3:I:37:PHE:CZ | 3:I:58:ILE:HD11 | 2.40 | 0.57 |
| 27:G:154:GLU:HG2 | 27:G:156:TYR:H | 1.69 | 0.57 |
| 2:B:176:A:O2' | 2:B:177:G:H5' | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 4:C:144:GLU:OE2 | 4:C:188:ARG:HG3 | 2.05 | 0.56 |
| 23:Q:97:ILE:HD11 | 23:Q:108:LEU:HD11 | 1.87 | 0.56 |
| 2:B:279:A:H2' | 2:B:280:U:H5' | 1.86 | 0.56 |
| 8:E:58:LYS:O | 8:E:60:TRP:N | 2.37 | 0.56 |
| 2:B:161:A:C3' | 2:B:162:U:H5'' | 2.33 | 0.56 |
| 30:Z:6:GLN:HE22 | 30:Z:50:ARG:N | 2.03 | 0.56 |
| 5:D:114:LYS:HD2 | 5:D:116:LYS:HZ2 | 1.68 | 0.56 |
| 14:V:80:HIS:HD2 | 14:V:83:LYS:H | 1.52 | 0.56 |
| 5:D:79:LEU:HD22 | 5:D:79:LEU:N | 2.20 | 0.56 |
| 2:B:1684:G:H2' | 2:B:1685:C:C6 | 2.40 | 0.56 |
| 28:R:27:ILE:HG13 | 28:R:33:VAL:HG11 | 1.87 | 0.56 |
| 2:B:710:U:H2' | 2:B:711:G:H8 | 1.70 | 0.56 |
| 2:B:1535:A:H3' | 2:B:1536:C:C6 | 2.40 | 0.56 |
| 31:W:39:GLN:HG2 | 31:W:40:ARG:N | 2.19 | 0.56 |
| 2:B:2385:C:H2' | 2:B:2386:A:C8 | 2.39 | 0.56 |
| 2:B:2543:G:H2' | 2:B:2544:G:C8 | 2.40 | 0.56 |
| 3:I:45:THR:CA | 3:I:48:ILE:HG22 | 2.34 | 0.56 |
| 21:N:47:VAL:C | 21:N:50:PRO:HD2 | 2.25 | 0.56 |
| 26:F:134:GLN:C | 26:F:136:ILE:H | 2.09 | 0.56 |
| 18:X:7:ARG:HA | 18:X:7:ARG:NE | 2.20 | 0.56 |
| 4:C:181:ARG:HH21 | 4:C:181:ARG:HG2 | 1.68 | 0.56 |
| 2:B:2292:U:H2' | 2:B:2293:G:C8 | 2.41 | 0.56 |
| 2:B:1947:C:O2' | 2:B:1948:G:H5' | 2.05 | 0.56 |
| 2:B:414:C:H2' | 2:B:415:A:C8 | 2.40 | 0.56 |
| 30:Z:45:ARG:O | 30:Z:46:PHE:HB2 | 2.04 | 0.56 |
| 5:D:106:LYS:O | 5:D:107:VAL:HB | 2.04 | 0.56 |
| 23:Q:96:ASP:C | 23:Q:98:ALA:H | 2.07 | 0.56 |
| 4:C:43:ASN:HB3 | 4:C:45:ASN:HD22 | 1.70 | 0.56 |
| 2:B:27:G:H1' | 2:B:513:A:H61 | 1.69 | 0.56 |
| 29:T:29:THR:CA | 29:T:86:THR:HA | 2.32 | 0.56 |
| 3:I:71:LYS:HB3 | 3:I:115:ASP:OD2 | 2.05 | 0.56 |
| 27:G:84:LYS:HG3 | 27:G:131:VAL:HB | 1.87 | 0.56 |
| 26:F:7:TYR:O | 26:F:12:VAL:HG23 | 2.05 | 0.56 |
| 19:H:7:ASP:CG | 19:H:8:LYS:H | 2.07 | 0.56 |
| 30:Z:11:ARG:HB3 | 30:Z:12:PRO:HD2 | 1.87 | 0.56 |
| 19:H:135:HIS:CG | 19:H:136:SER:H | 2.23 | 0.56 |
| 2:B:582:A:H2' | 2:B:583:G:H8 | 1.69 | 0.56 |
| 23:Q:24:TYR:O | 23:Q:27:ARG:HB2 | 2.05 | 0.56 |
| 2:B:2021:C:OP1 | 10:O:8:THR:HG21 | 2.05 | 0.56 |
| 2:B:416:U:H2' | 2:B:417:C:C6 | 2.40 | 0.56 |
| 17:M:105:MET:HB2 | 17:M:117:PHE:CE2 | 2.41 | 0.56 |
| 18:X:20:ASN:HA | 18:X:24:GLU:OE1 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:770:G:O2' | 2:B:771:G:H5' | 2.05 | 0.56 |
| 2:B:1818:U:N3 | 4:C:152:GLN:HB3 | 2.19 | 0.56 |
| 17:M:50:ARG:O | 17:M:53:MET:HB3 | 2.06 | 0.56 |
| 2:B:1061:U:O4' | 2:B:1070:A:H1' | 2.04 | 0.56 |
| 2:B:1061:U:H4' | 2:B:1070:A:O3' | 2.05 | 0.56 |
| 1:A:39:A:O2' | 1:A:40:U:H5' | 2.05 | 0.56 |
| 2:B:1098:A:H3' | 3:I:3:LYS:C | 2.25 | 0.56 |
| 31:W:58:LEU:HG | 31:W:79:ILE:HD12 | 1.87 | 0.56 |
| 29:T:11:LEU:CD2 | 29:T:46:ALA:HB1 | 2.35 | 0.56 |
| 26:F:32:LYS:NZ | 26:F:156:THR:HG21 | 2.20 | 0.56 |
| 20:J:18:VAL:CG1 | 20:J:54:ILE:HD11 | 2.34 | 0.56 |
| 8:E:145:ASP:OD1 | 8:E:166:LYS:HD2 | 2.06 | 0.56 |
| 2:B:483:A:H2' | 2:B:484:C:O4' | 2.05 | 0.56 |
| 2:B:616:A:H4' | 8:E:101:TYR:CE2 | 2.40 | 0.56 |
| 2:B:1351:C:O2' | 2:B:1571:A:H1' | 2.06 | 0.56 |
| 27:G:108:PHE:HD1 | 27:G:108:PHE:H | 1.52 | 0.56 |
| 2:B:966:G:H4' | 2:B:2272:U:O2 | 2.05 | 0.56 |
| 14:V:28:ALA:HB2 | 14:V:89:ILE:HD12 | 1.88 | 0.56 |
| 6:K:71:ARG:HA | 6:K:71:ARG:NE | 2.12 | 0.56 |
| 26:F:33:ILE:HD11 | 26:F:99:PHE:HB2 | 1.86 | 0.56 |
| 11:4:19:ARG:C | 11:4:21:GLY:H | 2.09 | 0.56 |
| 27:G:152:ARG:NH2 | 27:G:162:ARG:HA | 2.20 | 0.56 |
| 2:B:981:A:H2' | 2:B:982:C:H5'' | 1.88 | 0.56 |
| 2:B:222:A:H61 | 2:B:232:G:H1' | 1.70 | 0.56 |
| 2:B:102:U:H2' | 18:X:2:LYS:HE3 | 1.87 | 0.56 |
| 30:Z:40:VAL:HG13 | 30:Z:47:VAL:HG22 | 1.88 | 0.56 |
| 2:B:2547:A:H2' | 2:B:2548:U:C6 | 2.41 | 0.56 |
| 18:X:31:GLN:HG2 | 18:X:37:LEU:H | 1.69 | 0.56 |
| 20:J:45:THR:N | 20:J:46:PRO:HD3 | 2.20 | 0.56 |
| 31:W:17:ALA:CA | 31:W:35:ILE:HG23 | 2.33 | 0.56 |
| 2:B:138:U:H5' | 29:T:1:MET:N | 2.21 | 0.56 |
| 19:H:72:ILE:CG1 | 19:H:108:VAL:HG11 | 2.35 | 0.56 |
| 21:N:49:GLU:HB2 | 21:N:50:PRO:HD3 | 1.86 | 0.56 |
| 28:R:19:THR:HG22 | 28:R:97:LYS:HA | 1.87 | 0.56 |
| 2:B:17:G:H2' | 2:B:18:U:C6 | 2.40 | 0.56 |
| 14:V:6:ALA:HB3 | 14:V:65:VAL:HG12 | 1.87 | 0.56 |
| 26:F:141:ASP:HB2 | 26:F:144:LYS:HB2 | 1.88 | 0.56 |
| 2:B:102:U:H6 | 18:X:2:LYS:HE3 | 1.70 | 0.56 |
| 2:B:2266:A:H4' | 2:B:2267:A:C8 | 2.41 | 0.56 |
| 19:H:90:LEU:CB | 19:H:123:ARG:HA | 2.30 | 0.56 |
| 26:F:35:LEU:HD23 | 26:F:153:ILE:HG23 | 1.87 | 0.56 |
| 2:B:2329:U:H2' | 2:B:2330:G:C8 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 30:Z:4:VAL:HG12 | 30:Z:11:ARG:HG2 | 1.88 | 0.56 |
| 9:Y:7:THR:O | 9:Y:54:VAL:HA | 2.05 | 0.56 |
| 1:A:42:C:C5 | 26:F:65:LEU:HD22 | 2.41 | 0.56 |
| 4:C:20:ASN:ND2 | 4:C:23:LEU:HD13 | 2.21 | 0.56 |
| 2:B:633:A:O5' | 2:B:633:A:H8 | 1.88 | 0.56 |
| 21:N:9:GLN:HA | 21:N:17:ARG:NE | 2.21 | 0.56 |
| 16:L:17:LYS:HD2 | 16:L:19:LEU:HD11 | 1.87 | 0.56 |
| 2:B:2352:A:H2' | 2:B:2353:G:O4' | 2.06 | 0.56 |
| 2:B:297:G:OP1 | 25:U:91:LYS:HD3 | 2.05 | 0.56 |
| 27:G:8:VAL:HG11 | 27:G:49:LEU:N | 2.10 | 0.56 |
| 5:D:186:LEU:HD21 | 7:P:3:ILE:HD11 | 1.87 | 0.56 |
| 2:B:543:G:N2 | 2:B:545:U:H5' | 2.21 | 0.56 |
| 30:Z:32:ASN:O | 30:Z:33:LEU:O | 2.24 | 0.56 |
| 12:1:34:GLU:HB3 | 12:1:49:LYS:HD3 | 1.87 | 0.56 |
| 2:B:2142:A:H2' | 2:B:2143:C:C1' | 2.36 | 0.56 |
| 6:K:102:PRO:HD3 | 7:P:65:ASN:HB2 | 1.88 | 0.56 |
| 2:B:2895:G:H2' | 2:B:2896:C:H6 | 1.69 | 0.56 |
| 2:B:1412:U:H2' | 2:B:1413:A:H8 | 1.69 | 0.56 |
| 2:B:1033:U:C5 | 11:4:15:LYS:HE3 | 2.40 | 0.56 |
| 2:B:811:U:OP2 | 16:L:20:GLY:HA2 | 2.06 | 0.56 |
| 2:B:1098:A:C3' | 3:I:3:LYS:HA | 2.24 | 0.56 |
| 31:W:36:ILE:O | 31:W:39:GLN:HB3 | 2.06 | 0.56 |
| 23:Q:80:ASN:O | 23:Q:83:LYS:HB3 | 2.05 | 0.56 |
| 5:D:51:THR:CG2 | 5:D:76:GLY:HA3 | 2.35 | 0.56 |
| 7:P:50:ARG:HB2 | 7:P:56:SER:CB | 2.36 | 0.56 |
| 7:P:50:ARG:HB3 | 7:P:57:ALA:H | 1.71 | 0.56 |
| 26:F:24:VAL:O | 26:F:27:VAL:HG22 | 2.05 | 0.56 |
| 2:B:1442:U:H2' | 2:B:1443:U:C6 | 2.40 | 0.56 |
| 12:1:3:GLY:O | 12:1:4:ILE:HG12 | 2.06 | 0.56 |
| 19:H:135:HIS:CG | 19:H:136:SER:N | 2.73 | 0.56 |
| 2:B:666:A:H4' | 16:L:48:ARG:HD3 | 1.86 | 0.56 |
| 2:B:2756:U:C1' | 2:B:2757:A:H5'' | 2.35 | 0.56 |
| 2:B:1820:U:H4' | 2:B:1821:A:OP2 | 2.06 | 0.56 |
| 2:B:224:U:O4 | 2:B:420:C:H5' | 2.05 | 0.56 |
| 14:V:1:MET:CE | 14:V:2:PHE:H | 2.19 | 0.56 |
| 2:B:2693:G:O2' | 2:B:2694:G:H5' | 2.06 | 0.56 |
| 2:B:2537:U:H2' | 2:B:2538:C:C6 | 2.41 | 0.56 |
| 22:O:81:ARG:O | 22:O:84:GLU:HB3 | 2.06 | 0.56 |
| 27:G:66:THR:O | 27:G:70:LEU:HB2 | 2.06 | 0.56 |
| 7:P:75:THR:O | 7:P:80:VAL:HG11 | 2.05 | 0.56 |
| 24:S:73:LYS:CE | 24:S:74:ILE:H | 2.16 | 0.56 |
| 2:B:138:U:H2' | 2:B:140:C:C6 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:1199:U:H2' | 2:B:1200:C:C6 | 2.41 | 0.56 |
| 2:B:2840:C:H2' | 2:B:2841:C:C6 | 2.40 | 0.56 |
| 2:B:699:A:H4' | 2:B:1634:A:N7 | 2.21 | 0.56 |
| 2:B:1681:G:N3 | 2:B:1762:A:H2' | 2.20 | 0.56 |
| 2:B:782:A:N7 | 4:C:219:VAL:HG21 | 2.21 | 0.56 |
| 2:B:1098:A:C3' | 3:I:4:VAL:N | 2.69 | 0.55 |
| 28:R:3:ALA:O | 28:R:4:VAL:HG13 | 2.06 | 0.55 |
| 14:V:29:ILE:HG13 | 14:V:88:HIS:HE1 | 1.71 | 0.55 |
| 3:I:49:GLU:CB | 3:I:52:LEU:HD12 | 2.36 | 0.55 |
| 31:W:37:VAL:HG13 | 31:W:55:ASP:C | 2.26 | 0.55 |
| 2:B:1549:A:H2' | 2:B:1550:C:C6 | 2.40 | 0.55 |
| 6:K:115:ILE:HG23 | 6:K:116:ILE:N | 2.21 | 0.55 |
| 2:B:1242:U:H2' | 2:B:1243:C:C6 | 2.41 | 0.55 |
| 2:B:2751:G:OP2 | 27:G:2:ARG:HD2 | 2.06 | 0.55 |
| 2:B:118:A:OP2 | 2:B:119:A:H5'' | 2.05 | 0.55 |
| 2:B:2615:U:C2 | 10:O:3:GLN:HA | 2.42 | 0.55 |
| 31:W:51:GLY:HA3 | 31:W:59:PHE:HB3 | 1.87 | 0.55 |
| 19:H:94:ILE:O | 19:H:122:LEU:HD23 | 2.05 | 0.55 |
| 2:B:347:A:H2' | 2:B:348:A:H8 | 1.71 | 0.55 |
| 29:T:15:HIS:O | 29:T:16:VAL:C | 2.45 | 0.55 |
| 2:B:850:U:H2' | 2:B:851:C:C6 | 2.41 | 0.55 |
| 25:U:14:THR:O | 25:U:18:LYS:HG2 | 2.06 | 0.55 |
| 4:C:93:VAL:HG21 | 4:C:115:ILE:HD11 | 1.89 | 0.55 |
| 2:B:2800:A:H2' | 2:B:2801:G:C1' | 2.36 | 0.55 |
| 2:B:102:U:H2' | 18:X:2:LYS:NZ | 2.22 | 0.55 |
| 24:S:72:THR:CG2 | 24:S:108:SER:HB3 | 2.34 | 0.55 |
| 2:B:1000:A:H2' | 2:B:1001:A:C8 | 2.41 | 0.55 |
| 8:E:72:SER:C | 8:E:74:LYS:H | 2.08 | 0.55 |
| 26:F:130:GLY:HA2 | 26:F:152:ASP:HA | 1.88 | 0.55 |
| 27:G:71:LEU:HD22 | 27:G:74:MET:HE1 | 1.88 | 0.55 |
| 28:R:1:MET:HG3 | 28:R:101:ILE:HG21 | 1.88 | 0.55 |
| 29:T:11:LEU:HD22 | 29:T:11:LEU:N | 2.15 | 0.55 |
| 2:B:2810:A:H2' | 2:B:2811:G:O4' | 2.05 | 0.55 |
| 2:B:2557:G:H2' | 2:B:2558:C:H6 | 1.71 | 0.55 |
| 2:B:1240:U:O2' | 2:B:1241:A:H5'' | 2.06 | 0.55 |
| 2:B:1535:A:H3' | 2:B:1536:C:H6 | 1.70 | 0.55 |
| 18:X:18:LEU:O | 18:X:22:LEU:HB3 | 2.06 | 0.55 |
| 19:H:67:ALA:O | 19:H:70:GLU:HG3 | 2.06 | 0.55 |
| 2:B:2707:U:H2' | 2:B:2708:G:C8 | 2.41 | 0.55 |
| 27:G:7:PRO:O | 27:G:8:VAL:HG23 | 2.06 | 0.55 |
| 20:J:3:THR:HB | 20:J:44:TYR:CE1 | 2.41 | 0.55 |
| 2:B:559:G:H21 | 23:Q:51:GLN:NE2 | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 29:T:7:LEU:O | 29:T:7:LEU:HD13 | 2.07 | 0.55 |
| 2:B:1244:A:O2' | 2:B:1245:G:H5' | 2.06 | 0.55 |
| 24:S:31:GLN:C | 24:S:33:LEU:H | 2.10 | 0.55 |
| 27:G:166:GLU:CG | 27:G:168:VAL:HG23 | 2.35 | 0.55 |
| 27:G:88:LEU:O | 27:G:88:LEU:HD12 | 2.06 | 0.55 |
| 2:B:1593:A:H2' | 2:B:1594:U:C6 | 2.41 | 0.55 |
| 2:B:2849:U:N3 | 2:B:2867:G:C8 | 2.74 | 0.55 |
| 13:3:14:LYS:HD2 | 13:3:14:LYS:O | 2.05 | 0.55 |
| 23:Q:10:ARG:CZ | 23:Q:10:ARG:HB2 | 2.36 | 0.55 |
| 21:N:96:ARG:HH21 | 21:N:96:ARG:HG2 | 1.71 | 0.55 |
| 2:B:2103:C:H3' | 2:B:2104:C:C2 | 2.41 | 0.55 |
| 2:B:364:C:H2' | 2:B:365:U:C6 | 2.41 | 0.55 |
| 2:B:2008:C:H2' | 2:B:2009:A:C8 | 2.42 | 0.55 |
| 2:B:340:A:H2' | 2:B:341:C:O4' | 2.06 | 0.55 |
| 22:O:52:SER:O | 22:O:58:ILE:HD12 | 2.07 | 0.55 |
| 3:I:5:GLN:O | 3:I:6:ALA:HB3 | 2.06 | 0.55 |
| 2:B:1779:U:H5 | 2:B:1784:A:N7 | 2.05 | 0.55 |
| 2:B:2409:G:H2' | 2:B:2410:G:O4' | 2.06 | 0.55 |
| 2:B:2497:A:H5'' | 35:B:4118:HOH:O | 2.06 | 0.55 |
| 2:B:1192:G:O2' | 2:B:1193:G:H5' | 2.07 | 0.55 |
| 3:I:1:ALA:C | 3:I:2:LYS:HD2 | 2.27 | 0.55 |
| 16:L:77:ILE:HD11 | 16:L:95:LEU:HD13 | 1.88 | 0.55 |
| 29:T:68:LYS:O | 29:T:69:ARG:HB2 | 2.06 | 0.55 |
| 26:F:113:PHE:HZ | 26:F:175:PRO:HB2 | 1.70 | 0.55 |
| 2:B:851:C:H2' | 2:B:852:U:H6 | 1.71 | 0.55 |
| 25:U:64:ILE:HG13 | 25:U:65:GLN:N | 2.20 | 0.55 |
| 2:B:2645:G:H3' | 2:B:2646:C:C5' | 2.37 | 0.55 |
| 21:N:33:ILE:HD12 | 21:N:33:ILE:O | 2.07 | 0.55 |
| 2:B:528:A:C2 | 2:B:2043:C:H4' | 2.41 | 0.55 |
| 26:F:39:VAL:HG11 | 26:F:49:LEU:HA | 1.87 | 0.55 |
| 4:C:231:HIS:HA | 4:C:241:LYS:HE3 | 1.88 | 0.55 |
| 2:B:1429:G:H2' | 2:B:1430:G:C8 | 2.42 | 0.55 |
| 2:B:2564:A:OP1 | 2:B:2648:G:H4' | 2.07 | 0.55 |
| 5:D:125:TRP:CD2 | 5:D:160:LYS:HB3 | 2.41 | 0.55 |
| 2:B:2188:U:H2' | 2:B:2189:U:O4' | 2.06 | 0.55 |
| 2:B:2356:U:H5'' | 31:W:16:GLU:HG3 | 1.89 | 0.55 |
| 1:A:14:U:H4' | 1:A:70:C:O2 | 2.06 | 0.55 |
| 2:B:1623:G:O2' | 2:B:1624:U:H5' | 2.06 | 0.55 |
| 23:Q:91:ARG:CZ | 28:R:11:GLN:H | 2.20 | 0.55 |
| 28:R:39:LEU:CB | 28:R:53:PHE:HA | 2.37 | 0.55 |
| 26:F:116:LEU:HD23 | 26:F:176:PHE:N | 2.19 | 0.55 |
| 2:B:1203:U:H4' | 16:L:3:LEU:HD12 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:136:G:H2' | 2:B:137:U:C6 | 2.42 | 0.55 |
| 2:B:135:U:H2' | 2:B:136:G:O4' | 2.07 | 0.55 |
| 16:L:79:LEU:HG | 16:L:112:LEU:HA | 1.89 | 0.55 |
| 23:Q:30:VAL:O | 23:Q:33:VAL:HG22 | 2.06 | 0.55 |
| 2:B:532:A:N3 | 2:B:532:A:H2' | 2.22 | 0.55 |
| 21:N:34:ILE:O | 21:N:112:TYR:HA | 2.06 | 0.55 |
| 2:B:151:C:H2' | 2:B:152:A:H8 | 1.72 | 0.55 |
| 5:D:154:LYS:HG2 | 5:D:155:VAL:N | 2.21 | 0.55 |
| 2:B:2300:C:H2' | 2:B:2301:C:H6 | 1.71 | 0.55 |
| 2:B:2496:C:O2' | 2:B:2497:A:H5' | 2.07 | 0.55 |
| 5:D:36:GLN:HG3 | 5:D:36:GLN:O | 2.07 | 0.55 |
| 2:B:1013:C:H2' | 2:B:1014:A:H8 | 1.72 | 0.55 |
| 2:B:1847:A:H4' | 2:B:1848:A:C8 | 2.40 | 0.55 |
| 2:B:26:G:H1' | 2:B:514:A:N6 | 2.21 | 0.55 |
| 2:B:1098:A:O5' | 3:I:3:LYS:HG2 | 2.06 | 0.55 |
| 21:N:37:THR:OG1 | 21:N:40:LYS:HE2 | 2.06 | 0.55 |
| 27:G:17:LYS:HZ2 | 27:G:18:ILE:H | 1.54 | 0.55 |
| 19:H:95:GLY:H | 19:H:98:ASP:HB2 | 1.71 | 0.55 |
| 2:B:705:A:N6 | 2:B:726:G:H1' | 2.22 | 0.55 |
| 3:I:126:ARG:NH1 | 3:I:126:ARG:HB3 | 2.21 | 0.55 |
| 31:W:10:ARG:O | 31:W:11:ASN:HB2 | 2.07 | 0.55 |
| 27:G:94:ARG:HB2 | 27:G:127:GLN:HG2 | 1.88 | 0.55 |
| 2:B:582:A:H2' | 2:B:583:G:C8 | 2.41 | 0.55 |
| 4:C:173:LEU:HD13 | 4:C:173:LEU:N | 2.20 | 0.55 |
| 2:B:37:C:O2' | 2:B:38:A:H5' | 2.07 | 0.55 |
| 2:B:96:C:H4' | 18:X:41:HIS:CG | 2.41 | 0.55 |
| 2:B:1847:A:H4' | 2:B:1848:A:H8 | 1.72 | 0.55 |
| 19:H:129:GLU:HA | 19:H:143:ILE:HA | 1.89 | 0.55 |
| 2:B:1098:A:P | 3:I:3:LYS:HG2 | 2.46 | 0.55 |
| 31:W:23:LYS:HD2 | 31:W:24:ARG:H | 1.72 | 0.55 |
| 4:C:140:VAL:HG12 | 4:C:141:HIS:N | 2.20 | 0.55 |
| 2:B:557:C:H2' | 2:B:558:U:C6 | 2.41 | 0.55 |
| 23:Q:91:ARG:NH1 | 28:R:10:LYS:HB3 | 2.20 | 0.55 |
| 29:T:57:VAL:HG22 | 29:T:58:VAL:N | 2.19 | 0.55 |
| 3:I:54:ILE:HD13 | 3:I:55:PRO:N | 2.22 | 0.55 |
| 26:F:128:SER:HA | 26:F:154:THR:HA | 1.88 | 0.55 |
| 2:B:1140:C:H2' | 2:B:1141:U:H5' | 1.89 | 0.55 |
| 3:I:17:ALA:O | 3:I:18:ASN:CB | 2.55 | 0.55 |
| 2:B:850:U:H5'' | 9:Y:18:LYS:HD3 | 1.89 | 0.55 |
| 26:F:41:GLU:HB2 | 26:F:48:LEU:HD11 | 1.88 | 0.55 |
| 22:O:35:ILE:HG13 | 22:O:71:ALA:CB | 2.37 | 0.55 |
| 14:V:80:HIS:CD2 | 14:V:83:LYS:HB2 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:2393:U:O2' | 2:B:2394:C:H5' | 2.07 | 0.55 |
| 2:B:2633:G:H2' | 2:B:2634:A:O4' | 2.07 | 0.55 |
| 2:B:11:C:H2' | 2:B:12:U:H5' | 1.89 | 0.55 |
| 29:T:55:VAL:HA | 29:T:87:LEU:HA | 1.89 | 0.55 |
| 26:F:4:HIS:O | 26:F:7:TYR:HB3 | 2.07 | 0.55 |
| 31:W:37:VAL:O | 31:W:38:ARG:HG2 | 2.07 | 0.55 |
| 1:A:52:A:OP1 | 1:A:52:A:H4' | 2.06 | 0.55 |
| 27:G:167:VAL:HG21 | 27:G:169:ARG:HH12 | 1.72 | 0.55 |
| 21:N:17:ARG:HB2 | 21:N:17:ARG:HH21 | 1.71 | 0.55 |
| 4:C:149:LYS:HD3 | 4:C:152:GLN:HE22 | 1.72 | 0.55 |
| 2:B:2754:U:H6 | 2:B:2754:U:O5' | 1.90 | 0.55 |
| 2:B:1010:A:N3 | 2:B:1153:C:H1' | 2.21 | 0.55 |
| 2:B:997:G:O2' | 2:B:998:C:H5' | 2.06 | 0.55 |
| 31:W:21:GLY:N | 31:W:33:GLY:HA2 | 2.21 | 0.55 |
| 29:T:31:VAL:HA | 29:T:84:TYR:H | 1.71 | 0.55 |
| 4:C:91:ALA:HB2 | 4:C:105:ALA:HB2 | 1.88 | 0.55 |
| 26:F:161:SER:OG | 26:F:164:GLU:HG3 | 2.07 | 0.55 |
| 4:C:15:VAL:HG22 | 4:C:204:LEU:O | 2.07 | 0.55 |
| 2:B:95:A:H1' | 18:X:40:SER:OG | 2.06 | 0.55 |
| 6:K:104:THR:HB | 6:K:106:GLU:OE1 | 2.07 | 0.55 |
| 2:B:1433:A:H2' | 2:B:1434:A:O4' | 2.07 | 0.55 |
| 25:U:85:ARG:NE | 25:U:85:ARG:HA | 2.21 | 0.54 |
| 27:G:34:ARG:HH11 | 27:G:34:ARG:N | 1.98 | 0.54 |
| 23:Q:85:ALA:HB1 | 23:Q:111:LYS:HG3 | 1.89 | 0.54 |
| 2:B:283:G:H3' | 2:B:284:U:H5'' | 1.88 | 0.54 |
| 26:F:138:PRO:HA | 26:F:142:TYR:CE2 | 2.42 | 0.54 |
| 22:O:4:LYS:O | 22:O:8:ILE:HG13 | 2.07 | 0.54 |
| 23:Q:27:ARG:HA | 23:Q:33:VAL:HG23 | 1.89 | 0.54 |
| 2:B:2492:U:O2' | 2:B:2493:U:H5' | 2.07 | 0.54 |
| 20:J:21:THR:O | 20:J:62:VAL:HA | 2.08 | 0.54 |
| 2:B:2291:U:H2' | 2:B:2292:U:C6 | 2.42 | 0.54 |
| 2:B:80:G:HO2' | 2:B:294:A:H2 | 1.55 | 0.54 |
| 2:B:1656:C:H2' | 2:B:1657:U:H6 | 1.72 | 0.54 |
| 21:N:106:ASP:OD1 | 21:N:108:ALA:HB3 | 2.07 | 0.54 |
| 2:B:2265:U:H3' | 2:B:2266:A:C5' | 2.37 | 0.54 |
| 16:L:89:VAL:HA | 16:L:121:THR:O | 2.08 | 0.54 |
| 19:H:94:ILE:HG22 | 19:H:122:LEU:CB | 2.37 | 0.54 |
| 2:B:328:U:O3' | 25:U:65:GLN:HG3 | 2.07 | 0.54 |
| 2:B:2740:A:H2' | 2:B:2741:A:C8 | 2.43 | 0.54 |
| 7:P:19:PHE:CE2 | 7:P:25:VAL:HG11 | 2.43 | 0.54 |
| 2:B:2027:G:O2' | 2:B:2028:U:H5' | 2.07 | 0.54 |
| 5:D:35:THR:O | 5:D:36:GLN:HB3 | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 4:C:51:ARG:NH2 | 4:C:246:PRO:HG2 | 2.22 | 0.54 |
| 14:V:53:LYS:HD3 | 14:V:55:GLU:H | 1.71 | 0.54 |
| 7:P:77:SER:OG | 7:P:79:VAL:HG22 | 2.07 | 0.54 |
| 2:B:522:A:H2' | 2:B:523:C:C6 | 2.42 | 0.54 |
| 2:B:730:A:H5' | 35:B:4030:HOH:O | 2.06 | 0.54 |
| 2:B:374:A:N6 | 2:B:400:G:H1' | 2.22 | 0.54 |
| 16:L:119:PRO:HG3 | 16:L:138:ALA:O | 2.07 | 0.54 |
| 28:R:24:LYS:HA | 28:R:94:THR:CG2 | 2.36 | 0.54 |
| 2:B:1812:U:H2' | 2:B:1813:G:C8 | 2.42 | 0.54 |
| 19:H:89:LYS:HA | 19:H:123:ARG:O | 2.07 | 0.54 |
| 2:B:2306:C:C3' | 2:B:2307:G:H5' | 2.32 | 0.54 |
| 4:C:90:ILE:CD1 | 4:C:102:TYR:HB3 | 2.38 | 0.54 |
| 2:B:2179:C:C2' | 2:B:2179:C:O2 | 2.50 | 0.54 |
| 12:1:4:ILE:HD11 | 12:1:25:ASN:HD21 | 1.71 | 0.54 |
| 5:D:118:PHE:CE1 | 5:D:123:LYS:HD2 | 2.42 | 0.54 |
| 2:B:2866:U:H4' | 2:B:2867:G:H4' | 1.88 | 0.54 |
| 31:W:46:ALA:HB2 | 31:W:78:PHE:CD1 | 2.39 | 0.54 |
| 2:B:1939:U:O2 | 2:B:1967:C:H4' | 2.06 | 0.54 |
| 2:B:2231:U:O2' | 2:B:2232:C:H5' | 2.07 | 0.54 |
| 22:O:75:GLY:O | 22:O:78:VAL:HG23 | 2.08 | 0.54 |
| 2:B:1682:G:H2' | 2:B:1683:U:C6 | 2.42 | 0.54 |
| 24:S:96:ILE:HG23 | 24:S:96:ILE:O | 2.07 | 0.54 |
| 2:B:2704:C:H2' | 2:B:2705:A:O4' | 2.08 | 0.54 |
| 2:B:2785:C:H2' | 2:B:2786:U:H6 | 1.72 | 0.54 |
| 2:B:988:A:P | 9:Y:11:SER:HB3 | 2.48 | 0.54 |
| 19:H:53:GLU:O | 19:H:57:LYS:HB3 | 2.07 | 0.54 |
| 27:G:15:ASP:HB3 | 27:G:26:LYS:N | 2.09 | 0.54 |
| 7:P:4:ILE:O | 7:P:6:GLN:N | 2.40 | 0.54 |
| 26:F:109:ARG:HB3 | 26:F:135:ILE:CD1 | 2.37 | 0.54 |
| 27:G:174:LYS:HZ2 | 27:G:176:LYS:HG2 | 1.72 | 0.54 |
| 2:B:851:C:O2 | 9:Y:42:ALA:HB1 | 2.08 | 0.54 |
| 19:H:115:VAL:HG23 | 19:H:132:PHE:HA | 1.89 | 0.54 |
| 2:B:2141:G:H2' | 2:B:2142:A:C8 | 2.42 | 0.54 |
| 2:B:2808:G:HO2' | 2:B:2809:A:H8 | 1.55 | 0.54 |
| 11:4:36:ARG:HG2 | 11:4:37:GLN:H | 1.73 | 0.54 |
| 27:G:14:VAL:O | 27:G:16:VAL:HG23 | 2.07 | 0.54 |
| 2:B:591:U:H1' | 13:3:1:PRO:N | 2.22 | 0.54 |
| 2:B:208:C:H2' | 2:B:209:C:H6 | 1.71 | 0.54 |
| 2:B:2537:U:H2' | 2:B:2538:C:H6 | 1.72 | 0.54 |
| 8:E:73:ILE:O | 8:E:73:ILE:HG12 | 2.07 | 0.54 |
| 23:Q:57:ARG:NH1 | 23:Q:61:ILE:HD11 | 2.22 | 0.54 |
| 2:B:2182:U:H2' | 2:B:2183:A:C8 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:1460:U:H3' | 2:B:1461:C:H5' | 1.89 | 0.54 |
| 31:W:39:GLN:CG | 31:W:42:THR:HB | 2.37 | 0.54 |
| 25:U:86:PHE:CG | 25:U:87:GLU:N | 2.76 | 0.54 |
| 27:G:34:ARG:HD3 | 27:G:34:ARG:N | 2.23 | 0.54 |
| 2:B:1993:U:H4' | 5:D:133:THR:CG2 | 2.30 | 0.54 |
| 19:H:18:GLN:NE2 | 19:H:39:ALA:HB1 | 2.23 | 0.54 |
| 26:F:106:ALA:O | 26:F:135:ILE:HD13 | 2.08 | 0.54 |
| 19:H:13:GLY:O | 19:H:14:SER:HB2 | 2.07 | 0.54 |
| 27:G:145:ALA:HA | 27:G:148:ARG:HG3 | 1.89 | 0.54 |
| 28:R:71:LYS:HG3 | 28:R:72:VAL:N | 2.22 | 0.54 |
| 14:V:9:ARG:HH21 | 14:V:12:GLN:HA | 1.70 | 0.54 |
| 2:B:581:C:H2' | 2:B:582:A:H8 | 1.70 | 0.54 |
| 2:B:364:C:H2' | 2:B:365:U:H6 | 1.72 | 0.54 |
| 2:B:1190:G:O5' | 16:L:32:GLY:HA2 | 2.08 | 0.54 |
| 2:B:1846:G:H2' | 2:B:1847:A:O4' | 2.07 | 0.54 |
| 2:B:1322:A:C2' | 2:B:1323:C:H5' | 2.38 | 0.54 |
| 2:B:2053:G:O2' | 2:B:2054:A:H5' | 2.07 | 0.54 |
| 2:B:836:G:H2' | 2:B:837:C:C6 | 2.42 | 0.54 |
| 4:C:117:SER:CB | 4:C:128:THR:HB | 2.38 | 0.54 |
| 7:P:4:ILE:HA | 7:P:7:LEU:HD13 | 1.88 | 0.54 |
| 2:B:2443:C:H2' | 2:B:2444:G:C8 | 2.41 | 0.54 |
| 25:U:14:THR:HG23 | 25:U:15:GLY:N | 2.23 | 0.54 |
| 19:H:115:VAL:HG22 | 19:H:117:LEU:N | 2.22 | 0.54 |
| 24:S:16:LYS:O | 24:S:19:LEU:HB3 | 2.08 | 0.54 |
| 2:B:1508:A:H2' | 2:B:1509:A:C2 | 2.43 | 0.54 |
| 22:O:56:LYS:HE3 | 22:O:60:GLU:OE2 | 2.08 | 0.54 |
| 2:B:970:U:H1' | 2:B:985:C:P | 2.48 | 0.54 |
| 1:A:49:C:O3' | 22:O:68:LYS:HE3 | 2.07 | 0.54 |
| 22:O:51:ALA:HB1 | 22:O:77:ALA:HB3 | 1.88 | 0.54 |
| 2:B:870:U:O2' | 2:B:871:U:H5' | 2.08 | 0.54 |
| 14:V:53:LYS:HD3 | 14:V:55:GLU:HB2 | 1.90 | 0.54 |
| 2:B:2196:C:O2' | 2:B:2197:U:H5' | 2.07 | 0.54 |
| 19:H:27:ARG:HG2 | 19:H:27:ARG:HH21 | 1.73 | 0.54 |
| 2:B:2309:A:N6 | 26:F:75:GLY:HA3 | 2.23 | 0.54 |
| 4:C:189:ALA:C | 4:C:190:THR:HG23 | 2.26 | 0.54 |
| 2:B:1173:U:O5' | 2:B:1173:U:H6 | 1.91 | 0.54 |
| 2:B:496:G:H1' | 24:S:61:ASN:ND2 | 2.21 | 0.54 |
| 26:F:30:VAL:HG21 | 26:F:96:TRP:NE1 | 2.20 | 0.54 |
| 9:Y:9:THR:HB | 9:Y:53:MET:O | 2.07 | 0.54 |
| 16:L:3:LEU:O | 16:L:5:THR:N | 2.41 | 0.54 |
| 19:H:131:SER:HB2 | 19:H:141:LYS:HG3 | 1.90 | 0.54 |
| 17:M:37:GLY:HA3 | 17:M:127:LYS:NZ | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2678:C:H2' | 2:B:2679:A:C8 | 2.42 | 0.54 |
| 17:M:59:ARG:NH1 | 17:M:60:GLN:HB3 | 2.22 | 0.54 |
| 14:V:62:THR:HG22 | 14:V:71:LYS:NZ | 2.22 | 0.54 |
| 2:B:65:U:H2' | 2:B:66:C:H6 | 1.72 | 0.54 |
| 13:3:50:SER:C | 13:3:52:GLY:H | 2.11 | 0.54 |
| 1:A:13:G:H1 | 1:A:69:G:HO2' | 1.56 | 0.54 |
| 25:U:98:ASN:OD1 | 25:U:100:GLU:HB2 | 2.08 | 0.54 |
| 2:B:950:G:H2' | 2:B:951:C:C6 | 2.43 | 0.54 |
| 2:B:2450:A:O2' | 2:B:2451:A:H5' | 2.07 | 0.54 |
| 18:X:1:MET:HA | 18:X:4:LYS:HE2 | 1.89 | 0.54 |
| 28:R:79:ARG:C | 28:R:81:LYS:H | 2.11 | 0.54 |
| 3:I:2:LYS:NZ | 3:I:2:LYS:HB3 | 2.23 | 0.54 |
| 21:N:38:LEU:HG | 21:N:42:LYS:HD2 | 1.89 | 0.54 |
| 27:G:9:VAL:O | 27:G:11:PRO:HD3 | 2.07 | 0.54 |
| 19:H:90:LEU:HD21 | 19:H:94:ILE:HB | 1.89 | 0.54 |
| 26:F:107:VAL:N | 26:F:108:PRO:CD | 2.71 | 0.54 |
| 26:F:168:LEU:O | 26:F:170:ALA:N | 2.41 | 0.54 |
| 26:F:3:LEU:HD11 | 26:F:172:PHE:CD1 | 2.43 | 0.54 |
| 25:U:78:LYS:CD | 25:U:79:ALA:H | 2.21 | 0.54 |
| 2:B:2598:A:OP1 | 4:C:233:GLY:HA2 | 2.08 | 0.54 |
| 2:B:1727:C:H2' | 2:B:1728:C:O4' | 2.07 | 0.54 |
| 26:F:141:ASP:CB | 26:F:144:LYS:HB2 | 2.38 | 0.54 |
| 2:B:937:C:H2' | 2:B:938:G:C8 | 2.43 | 0.54 |
| 2:B:1273:U:H4' | 2:B:1275:A:OP2 | 2.08 | 0.54 |
| 18:X:20:ASN:O | 18:X:24:GLU:HB3 | 2.08 | 0.54 |
| 6:K:79:PHE:HZ | 6:K:104:THR:HG23 | 1.73 | 0.54 |
| 2:B:1126:A:H8 | 2:B:1126:A:OP1 | 1.91 | 0.54 |
| 11:4:27:CYS:SG | 11:4:29:ALA:HB3 | 2.48 | 0.54 |
| 2:B:511:U:H5' | 2:B:1236:G:OP1 | 2.07 | 0.54 |
| 2:B:657:U:H2' | 2:B:658:U:C6 | 2.43 | 0.54 |
| 5:D:53:GLY:C | 5:D:76:GLY:HA2 | 2.28 | 0.54 |
| 14:V:32:GLY:O | 14:V:93:ARG:HD2 | 2.07 | 0.54 |
| 14:V:69:GLU:C | 14:V:70:ILE:HD13 | 2.27 | 0.54 |
| 17:M:42:THR:O | 17:M:44:ARG:N | 2.38 | 0.54 |
| 26:F:60:SER:HB3 | 26:F:62:GLN:OE1 | 2.07 | 0.54 |
| 20:J:58:ASN:HA | 20:J:127:GLY:CA | 2.35 | 0.54 |
| 2:B:1104:C:H2' | 2:B:1105:U:C6 | 2.43 | 0.54 |
| 27:G:88:LEU:HB3 | 27:G:161:VAL:HG13 | 1.90 | 0.54 |
| 21:N:28:LEU:O | 21:N:28:LEU:HD22 | 2.08 | 0.54 |
| 4:C:239:PHE:HD1 | 4:C:241:LYS:H | 1.56 | 0.54 |
| 2:B:2359:C:H2' | 2:B:2360:G:C8 | 2.43 | 0.54 |
| 2:B:2066:C:O2' | 2:B:2067:G:H5' | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 19:H:80:ILE:HG12 | 19:H:147:VAL:H | 1.73 | 0.54 |
| 22:O:79:ALA:HA | 22:O:115:LEU:HD23 | 1.88 | 0.54 |
| 2:B:1957:C:H2' | 2:B:1958:C:C6 | 2.43 | 0.54 |
| 16:L:18:ARG:C | 16:L:19:LEU:HD12 | 2.28 | 0.54 |
| 2:B:2785:C:H2' | 2:B:2786:U:C6 | 2.43 | 0.54 |
| 4:C:119:VAL:HG13 | 4:C:133:ASN:HD21 | 1.72 | 0.54 |
| 2:B:228:C:H4' | 2:B:229:C:H5'' | 1.90 | 0.54 |
| 2:B:39:G:H2' | 2:B:40:U:C6 | 2.43 | 0.54 |
| 18:X:39:GLN:HB2 | 18:X:42:LEU:HD22 | 1.89 | 0.54 |
| 28:R:25:LEU:H | 28:R:94:THR:HG21 | 1.73 | 0.54 |
| 25:U:11:ILE:HD13 | 25:U:11:ILE:O | 2.07 | 0.54 |
| 14:V:61:LEU:HD11 | 14:V:74:ALA:HB2 | 1.88 | 0.54 |
| 4:C:243:PRO:O | 4:C:250:GLN:HA | 2.08 | 0.54 |
| 13:3:49:VAL:HG21 | 13:3:54:LEU:HD13 | 1.90 | 0.54 |
| 2:B:2774:C:OP1 | 5:D:169:ARG:HG3 | 2.08 | 0.54 |
| 2:B:1459:G:H4' | 2:B:1461:C:N4 | 2.23 | 0.54 |
| 2:B:1215:G:O2' | 2:B:1216:G:H5' | 2.08 | 0.54 |
| 2:B:1854:A:N6 | 2:B:1888:G:H1' | 2.22 | 0.54 |
| 2:B:2671:G:H2' | 2:B:2672:U:C6 | 2.42 | 0.54 |
| 20:J:19:ASP:OD2 | 20:J:58:ASN:HB2 | 2.08 | 0.53 |
| 2:B:2666:C:O2 | 2:B:2666:C:O4' | 2.25 | 0.53 |
| 2:B:850:U:O3' | 9:Y:22:THR:HG22 | 2.07 | 0.53 |
| 19:H:96:THR:HG23 | 19:H:97:ARG:N | 2.22 | 0.53 |
| 2:B:636:G:O5' | 16:L:128:THR:HG22 | 2.07 | 0.53 |
| 23:Q:10:ARG:NH1 | 23:Q:10:ARG:HB2 | 2.23 | 0.53 |
| 2:B:709:U:H2' | 2:B:710:U:C6 | 2.43 | 0.53 |
| 4:C:6:LYS:O | 4:C:8:THR:HG23 | 2.08 | 0.53 |
| 27:G:79:THR:HG22 | 27:G:80:GLU:HG2 | 1.90 | 0.53 |
| 31:W:67:LYS:O | 31:W:68:PHE:HB2 | 2.07 | 0.53 |
| 20:J:88:THR:HG22 | 20:J:91:GLU:HG3 | 1.90 | 0.53 |
| 2:B:1274:A:N3 | 2:B:1297:C:H1' | 2.23 | 0.53 |
| 3:I:1:ALA:CB | 3:I:2:LYS:HD2 | 2.38 | 0.53 |
| 4:C:143:VAL:HG12 | 4:C:144:GLU:H | 1.72 | 0.53 |
| 20:J:25:LEU:HD22 | 20:J:26:GLY:N | 2.24 | 0.53 |
| 23:Q:59:LEU:HD13 | 23:Q:60:TRP:N | 2.23 | 0.53 |
| 29:T:55:VAL:HG22 | 29:T:87:LEU:HD23 | 1.90 | 0.53 |
| 26:F:71:LYS:O | 26:F:72:SER:HB3 | 2.07 | 0.53 |
| 31:W:37:VAL:CG1 | 31:W:38:ARG:H | 2.18 | 0.53 |
| 2:B:2720:U:H2' | 2:B:2721:A:C8 | 2.43 | 0.53 |
| 2:B:1438:U:H2' | 2:B:1439:A:O4' | 2.09 | 0.53 |
| 16:L:6:LEU:CD2 | 16:L:6:LEU:H | 2.18 | 0.53 |
| 8:E:119:ILE:HD11 | 8:E:185:LYS:HZ1 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2680:U:OP2 | 5:D:114:LYS:HB3 | 2.08 | 0.53 |
| 2:B:64:A:H2' | 2:B:65:U:C6 | 2.43 | 0.53 |
| 7:P:112:ARG:HB2 | 7:P:112:ARG:HH11 | 1.74 | 0.53 |
| 29:T:50:LEU:C | 29:T:52:GLU:H | 2.10 | 0.53 |
| 2:B:458:G:O2' | 15:2:39:ARG:HD2 | 2.08 | 0.53 |
| 2:B:2026:U:H2' | 2:B:2027:G:C8 | 2.44 | 0.53 |
| 2:B:1777:U:O2' | 2:B:1778:U:H5' | 2.09 | 0.53 |
| 24:S:12:SER:O | 24:S:13:SER:HB3 | 2.08 | 0.53 |
| 4:C:1:ALA:HB3 | 4:C:19:VAL:HG23 | 1.90 | 0.53 |
| 31:W:50:VAL:HG23 | 31:W:61:LYS:CD | 2.35 | 0.53 |
| 16:L:95:LEU:O | 16:L:100:ILE:HG22 | 2.08 | 0.53 |
| 2:B:78:U:H2' | 2:B:79:C:H6 | 1.72 | 0.53 |
| 29:T:14:PRO:HA | 29:T:32:LEU:CB | 2.38 | 0.53 |
| 29:T:43:ILE:O | 29:T:46:ALA:HB3 | 2.08 | 0.53 |
| 26:F:11:VAL:HG12 | 26:F:12:VAL:N | 2.19 | 0.53 |
| 30:Z:67:VAL:O | 30:Z:71:LEU:HD23 | 2.08 | 0.53 |
| 29:T:50:LEU:HD22 | 29:T:50:LEU:N | 2.23 | 0.53 |
| 2:B:303:G:H2' | 2:B:304:U:C6 | 2.43 | 0.53 |
| 2:B:184:C:H2' | 2:B:185:G:C8 | 2.43 | 0.53 |
| 29:T:12:ARG:HB3 | 29:T:12:ARG:NH1 | 2.23 | 0.53 |
| 2:B:235:U:H2' | 2:B:236:C:H6 | 1.73 | 0.53 |
| 2:B:2024:G:O2' | 2:B:2025:C:H5' | 2.08 | 0.53 |
| 2:B:2309:A:H61 | 26:F:75:GLY:HA3 | 1.73 | 0.53 |
| 7:P:110:LYS:HD2 | 7:P:110:LYS:N | 2.23 | 0.53 |
| 3:I:63:ASP:O | 3:I:64:ARG:HB2 | 2.07 | 0.53 |
| 30:Z:37:ARG:HA | 30:Z:48:THR:HB | 1.89 | 0.53 |
| 2:B:2660:A:H2' | 2:B:2661:G:O4' | 2.08 | 0.53 |
| 2:B:1450:G:H21 | 2:B:1452:G:H1 | 1.56 | 0.53 |
| 27:G:59:ASP:O | 27:G:63:GLN:HB2 | 2.08 | 0.53 |
| 16:L:77:ILE:HD11 | 16:L:95:LEU:HD22 | 1.91 | 0.53 |
| 28:R:49:ILE:HD13 | 28:R:53:PHE:N | 2.23 | 0.53 |
| 5:D:13:ARG:HH12 | 7:P:74:GLN:NE2 | 2.05 | 0.53 |
| 17:M:19:GLY:N | 17:M:38:ARG:HH12 | 1.98 | 0.53 |
| 6:K:71:ARG:CG | 6:K:105:ARG:HH21 | 2.21 | 0.53 |
| 2:B:347:A:H2' | 2:B:348:A:C8 | 2.43 | 0.53 |
| 2:B:91:A:H1' | 2:B:92:U:C6 | 2.43 | 0.53 |
| 4:C:94:LEU:HA | 4:C:100:ARG:HB3 | 1.90 | 0.53 |
| 25:U:12:VAL:HA | 25:U:69:VAL:HA | 1.89 | 0.53 |
| 2:B:878:A:H5' | 2:B:900:A:H61 | 1.73 | 0.53 |
| 2:B:1197:G:H2' | 2:B:1198:U:C6 | 2.43 | 0.53 |
| 2:B:1464:G:H2' | 2:B:1465:G:C8 | 2.43 | 0.53 |
| 2:B:49:A:H5'' | 2:B:51:G:O4' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:D:110:THR:HG23 | 5:D:171:THR:HB | 1.89 | 0.53 |
| 2:B:2332:C:H5' | 31:W:40:ARG:HB3 | 1.90 | 0.53 |
| 27:G:30:GLY:CA | 27:G:78:VAL:HA | 2.37 | 0.53 |
| 28:R:49:ILE:O | 28:R:49:ILE:HD12 | 2.08 | 0.53 |
| 3:I:129:GLU:HB3 | 3:I:133:ARG:HH12 | 1.73 | 0.53 |
| 2:B:1727:C:H2' | 2:B:1728:C:H6 | 1.73 | 0.53 |
| 2:B:1790:C:O2' | 4:C:207:ALA:HB2 | 2.08 | 0.53 |
| 18:X:29:ARG:HH21 | 18:X:29:ARG:HB2 | 1.73 | 0.53 |
| 24:S:84:ARG:HB3 | 24:S:96:ILE:HG23 | 1.89 | 0.53 |
| 29:T:64:LYS:H | 29:T:64:LYS:HD2 | 1.74 | 0.53 |
| 5:D:101:PHE:O | 5:D:180:VAL:HG11 | 2.09 | 0.53 |
| 29:T:62:VAL:HG12 | 29:T:63:VAL:H | 1.73 | 0.53 |
| 2:B:1909:C:O2' | 2:B:1910:G:H5' | 2.08 | 0.53 |
| 2:B:1475:G:H4' | 2:B:1476:U:O5' | 2.08 | 0.53 |
| 27:G:17:LYS:HZ2 | 27:G:18:ILE:N | 2.07 | 0.53 |
| 14:V:28:ALA:HA | 14:V:88:HIS:ND1 | 2.24 | 0.53 |
| 2:B:350:G:H2' | 2:B:351:C:C6 | 2.44 | 0.53 |
| 19:H:12:LEU:HD21 | 19:H:25:TYR:HE2 | 1.73 | 0.53 |
| 23:Q:65:ASN:CB | 23:Q:75:TYR:HB2 | 2.38 | 0.53 |
| 9:Y:9:THR:OG1 | 9:Y:55:LYS:HB2 | 2.09 | 0.53 |
| 9:Y:23:LEU:HD13 | 9:Y:28:LEU:HB2 | 1.90 | 0.53 |
| 14:V:56:PHE:O | 14:V:61:LEU:HD21 | 2.09 | 0.53 |
| 2:B:979:A:H2' | 2:B:982:C:N4 | 2.23 | 0.53 |
| 20:J:104:ALA:O | 20:J:108:MET:HG2 | 2.08 | 0.53 |
| 20:J:72:LYS:CB | 20:J:89:PHE:HB2 | 2.39 | 0.53 |
| 2:B:1407:G:H2' | 2:B:1408:G:H8 | 1.74 | 0.53 |
| 2:B:2896:C:H2' | 2:B:2897:U:C6 | 2.44 | 0.53 |
| 2:B:2896:C:H2' | 2:B:2897:U:H6 | 1.72 | 0.53 |
| 27:G:40:VAL:HG22 | 27:G:64:ALA:HA | 1.91 | 0.53 |
| 2:B:1013:C:H2' | 2:B:1014:A:C8 | 2.43 | 0.53 |
| 2:B:526:A:N6 | 2:B:2626:C:H4' | 2.23 | 0.53 |
| 2:B:2835:A:H61 | 2:B:2878:U:H2' | 1.74 | 0.53 |
| 20:J:1:MET:HG2 | 20:J:2:LYS:HG2 | 1.91 | 0.53 |
| 2:B:2074:U:H2' | 2:B:2075:U:C6 | 2.44 | 0.53 |
| 2:B:1425:G:H2' | 2:B:1426:G:C8 | 2.44 | 0.53 |
| 31:W:49:ASN:CB | 31:W:60:ALA:HA | 2.28 | 0.53 |
| 23:Q:105:PHE:HA | 23:Q:108:LEU:CD1 | 2.36 | 0.53 |
| 23:Q:93:ILE:O | 23:Q:96:ASP:HB3 | 2.09 | 0.53 |
| 14:V:26:PHE:CE2 | 14:V:44:HIS:HA | 2.43 | 0.53 |
| 2:B:30:G:OP1 | 23:Q:4:LYS:HG2 | 2.09 | 0.53 |
| 2:B:704:G:H2' | 2:B:726:G:N2 | 2.15 | 0.53 |
| 2:B:1244:A:H5'' | 16:L:8:PRO:CD | 2.32 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:1591:A:H2' | 2:B:1592:C:O4' | 2.09 | 0.53 |
| 2:B:2867:G:C2' | 2:B:2867:G:N3 | 2.72 | 0.53 |
| 3:I:85:ILE:CD1 | 3:I:137:LEU:HD21 | 2.38 | 0.53 |
| 2:B:1568:G:H4' | 4:C:58:LYS:HB3 | 1.90 | 0.53 |
| 27:G:47:ASN:OD1 | 27:G:48:THR:HG23 | 2.08 | 0.53 |
| 2:B:1166:G:H2' | 2:B:1167:C:H6 | 1.72 | 0.53 |
| 5:D:124:ARG:HA | 5:D:165:MET:CE | 2.39 | 0.53 |
| 2:B:2339:C:H2' | 2:B:2340:A:C8 | 2.43 | 0.53 |
| 14:V:46:LYS:HD2 | 14:V:46:LYS:N | 2.24 | 0.53 |
| 4:C:18:VAL:HG13 | 4:C:18:VAL:O | 2.08 | 0.53 |
| 18:X:45:GLN:O | 18:X:47:ARG:N | 2.41 | 0.53 |
| 26:F:66:ILE:HD11 | 26:F:83:PRO:HB3 | 1.91 | 0.53 |
| 28:R:10:LYS:N | 28:R:10:LYS:HD2 | 2.24 | 0.53 |
| 29:T:13:ALA:O | 29:T:32:LEU:HB2 | 2.08 | 0.53 |
| 3:I:52:LEU:HD22 | 3:I:81:LYS:HD3 | 1.90 | 0.53 |
| 2:B:443:A:C8 | 8:E:40:ARG:HD3 | 2.44 | 0.53 |
| 2:B:852:U:H2' | 2:B:853:C:C6 | 2.44 | 0.53 |
| 25:U:78:LYS:HZ2 | 25:U:78:LYS:HA | 1.73 | 0.53 |
| 2:B:233:A:N6 | 2:B:428:A:N6 | 2.57 | 0.53 |
| 2:B:96:C:H4' | 18:X:41:HIS:CE1 | 2.43 | 0.53 |
| 2:B:673:C:H5'' | 8:E:76:PRO:HD2 | 1.90 | 0.53 |
| 2:B:438:G:H2' | 2:B:439:A:C8 | 2.44 | 0.53 |
| 8:E:137:LYS:O | 8:E:141:MET:HG3 | 2.08 | 0.53 |
| 6:K:35:VAL:HG12 | 6:K:69:VAL:CG2 | 2.38 | 0.53 |
| 23:Q:56:PHE:HA | 23:Q:59:LEU:HB3 | 1.90 | 0.53 |
| 7:P:4:ILE:C | 7:P:6:GLN:N | 2.61 | 0.53 |
| 12:1:28:THR:C | 12:1:30:PRO:HD3 | 2.29 | 0.53 |
| 2:B:580:U:O3' | 23:Q:30:VAL:HG13 | 2.08 | 0.53 |
| 2:B:592:A:H2' | 2:B:593:U:H6 | 1.74 | 0.53 |
| 22:O:88:LYS:HG2 | 22:O:89:ASP:H | 1.73 | 0.53 |
| 2:B:2471:A:O2' | 2:B:2472:G:C8 | 2.56 | 0.53 |
| 4:C:156:SER:HB3 | 4:C:159:THR:HG21 | 1.91 | 0.53 |
| 2:B:639:U:H2' | 2:B:640:C:H6 | 1.73 | 0.53 |
| 2:B:1198:U:H2' | 2:B:1199:U:H6 | 1.74 | 0.53 |
| 2:B:2322:A:N6 | 2:B:2333:A:N6 | 2.57 | 0.53 |
| 5:D:55:LYS:H | 5:D:76:GLY:H | 1.57 | 0.53 |
| 27:G:97:VAL:HA | 27:G:102:ILE:HA | 1.91 | 0.53 |
| 24:S:29:VAL:CA | 24:S:32:ALA:HB3 | 2.37 | 0.53 |
| 3:I:32:VAL:HG22 | 3:I:60:VAL:CG2 | 2.39 | 0.53 |
| 2:B:361:G:O2' | 2:B:362:A:H5' | 2.09 | 0.53 |
| 19:H:135:HIS:HB3 | 19:H:138:VAL:CB | 2.37 | 0.53 |
| 2:B:1590:A:H2' | 2:B:1591:A:H8 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:2078:C:H2' | 2:B:2079:U:H6 | 1.74 | 0.53 |
| 2:B:1736:U:H2' | 2:B:1737:G:O4' | 2.09 | 0.53 |
| 2:B:937:C:H2' | 2:B:938:G:H8 | 1.73 | 0.53 |
| 2:B:1771:C:H2' | 2:B:1772:A:C8 | 2.43 | 0.53 |
| 2:B:318:C:H2' | 2:B:319:G:H8 | 1.74 | 0.53 |
| 2:B:1106:G:H2' | 2:B:1107:G:H8 | 1.74 | 0.53 |
| 4:C:209:ALA:HA | 4:C:212:TRP:CE2 | 2.44 | 0.53 |
| 2:B:2445:G:O2' | 2:B:2446:G:H5' | 2.09 | 0.53 |
| 2:B:354:A:H2' | 2:B:355:U:C6 | 2.44 | 0.53 |
| 2:B:2776:A:H4' | 2:B:2777:G:H5'' | 1.91 | 0.53 |
| 2:B:1291:C:O2' | 2:B:1292:G:H5' | 2.08 | 0.53 |
| 16:L:125:LEU:HB2 | 16:L:143:GLU:OE2 | 2.08 | 0.52 |
| 5:D:51:THR:HG22 | 5:D:52:THR:H | 1.74 | 0.52 |
| 4:C:83:ASP:HB2 | 4:C:90:ILE:HB | 1.91 | 0.52 |
| 24:S:46:LEU:O | 24:S:50:VAL:HG23 | 2.09 | 0.52 |
| 26:F:137:PHE:O | 26:F:139:GLU:N | 2.42 | 0.52 |
| 21:N:47:VAL:O | 21:N:51:LEU:HD13 | 2.10 | 0.52 |
| 5:D:62:LYS:HB2 | 5:D:63:PRO:HD3 | 1.91 | 0.52 |
| 2:B:170:U:H2' | 2:B:171:U:H6 | 1.74 | 0.52 |
| 4:C:57:HIS:CG | 4:C:58:LYS:N | 2.76 | 0.52 |
| 2:B:2065:C:H2' | 2:B:2066:C:C6 | 2.44 | 0.52 |
| 19:H:77:THR:HA | 19:H:143:ILE:O | 2.08 | 0.52 |
| 2:B:1309:G:H4' | 15:2:7:PRO:HB2 | 1.91 | 0.52 |
| 26:F:14:LYS:O | 26:F:18:GLU:HB2 | 2.10 | 0.52 |
| 31:W:47:GLY:HA3 | 31:W:80:SER:HB2 | 1.90 | 0.52 |
| 2:B:2737:G:H2' | 2:B:2738:A:C8 | 2.44 | 0.52 |
| 2:B:2389:G:H5'' | 2:B:2390:U:H5' | 1.91 | 0.52 |
| 16:L:92:LEU:H | 16:L:92:LEU:HD23 | 1.74 | 0.52 |
| 21:N:8:ARG:HH21 | 21:N:39:PRO:HB3 | 1.72 | 0.52 |
| 27:G:30:GLY:HA3 | 27:G:78:VAL:HG12 | 1.90 | 0.52 |
| 23:Q:94:LEU:C | 23:Q:96:ASP:H | 2.13 | 0.52 |
| 29:T:30:ILE:O | 29:T:85:VAL:HG23 | 2.09 | 0.52 |
| 26:F:78:ILE:N | 26:F:78:ILE:HD12 | 2.25 | 0.52 |
| 17:M:41:LEU:O | 17:M:94:ALA:N | 2.41 | 0.52 |
| 2:B:1138:G:H2' | 2:B:1139:G:O4' | 2.10 | 0.52 |
| 2:B:849:A:H2' | 2:B:850:U:C6 | 2.44 | 0.52 |
| 2:B:2675:A:N1 | 2:B:2732:G:O6 | 2.42 | 0.52 |
| 21:N:32:GLU:O | 21:N:114:GLU:HA | 2.09 | 0.52 |
| 2:B:1387:A:C4' | 2:B:1469:A:H1' | 2.39 | 0.52 |
| 2:B:2037:A:H2' | 2:B:2038:G:C8 | 2.45 | 0.52 |
| 2:B:898:C:H2' | 2:B:899:A:H5'' | 1.91 | 0.52 |
| 2:B:794:A:H2' | 2:B:795:C:H6 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:686:U:O2 | 15:2:8:SER:HB3 | 2.09 | 0.52 |
| 4:C:28:PRO:HG2 | 4:C:33:LEU:HD11 | 1.90 | 0.52 |
| 2:B:693:A:H2' | 2:B:694:U:C6 | 2.44 | 0.52 |
| 2:B:753:A:O2' | 2:B:754:U:H5' | 2.09 | 0.52 |
| 2:B:1099:G:O5' | 3:I:4:VAL:HG12 | 2.10 | 0.52 |
| 2:B:1100:C:H2' | 2:B:1101:U:C6 | 2.45 | 0.52 |
| 2:B:2369:A:O2' | 2:B:2370:G:H5' | 2.09 | 0.52 |
| 16:L:95:LEU:HB3 | 16:L:100:ILE:CG2 | 2.40 | 0.52 |
| 20:J:3:THR:HB | 20:J:44:TYR:HE1 | 1.75 | 0.52 |
| 14:V:42:LEU:CD1 | 14:V:47:VAL:HG21 | 2.33 | 0.52 |
| 29:T:87:LEU:HB2 | 29:T:91:GLN:HG2 | 1.90 | 0.52 |
| 25:U:20:LYS:HB2 | 25:U:20:LYS:NZ | 2.23 | 0.52 |
| 25:U:72:PHE:HA | 25:U:78:LYS:O | 2.10 | 0.52 |
| 2:B:2679:A:O2' | 2:B:2680:U:H5' | 2.09 | 0.52 |
| 26:F:148:VAL:O | 26:F:149:ARG:HG2 | 2.09 | 0.52 |
| 4:C:255:LYS:C | 4:C:257:ARG:H | 2.12 | 0.52 |
| 2:B:1030:C:O2' | 2:B:1031:G:H5' | 2.09 | 0.52 |
| 2:B:1640:A:H8 | 2:B:1640:A:H5' | 1.74 | 0.52 |
| 27:G:10:VAL:HG23 | 27:G:48:THR:HA | 1.91 | 0.52 |
| 2:B:1509:A:C3' | 2:B:1510:G:H5' | 2.40 | 0.52 |
| 2:B:1937:A:N7 | 2:B:1939:U:H2' | 2.24 | 0.52 |
| 2:B:814:C:H2' | 2:B:815:C:H6 | 1.74 | 0.52 |
| 2:B:1674:G:N2 | 2:B:1677:A:N1 | 2.54 | 0.52 |
| 2:B:1322:A:H2' | 2:B:1323:C:H5' | 1.92 | 0.52 |
| 2:B:1041:G:H2' | 2:B:1042:G:H8 | 1.73 | 0.52 |
| 16:L:47:ARG:HG3 | 16:L:50:PHE:HB2 | 1.91 | 0.52 |
| 2:B:2662:A:H2' | 2:B:2663:G:O4' | 2.10 | 0.52 |
| 2:B:912:C:O2' | 2:B:913:U:H5' | 2.10 | 0.52 |
| 27:G:17:LYS:NZ | 27:G:18:ILE:H | 2.07 | 0.52 |
| 28:R:4:VAL:HG21 | 28:R:40:MET:HB2 | 1.92 | 0.52 |
| 5:D:10:GLY:O | 5:D:11:MET:HB2 | 2.09 | 0.52 |
| 17:M:19:GLY:H | 17:M:38:ARG:NH1 | 1.95 | 0.52 |
| 29:T:11:LEU:HD11 | 29:T:46:ALA:HB3 | 1.92 | 0.52 |
| 26:F:78:ILE:HA | 26:F:82:TYR:CD1 | 2.45 | 0.52 |
| 2:B:1201:U:H2' | 2:B:1202:G:C8 | 2.45 | 0.52 |
| 1:A:32:U:H1' | 1:A:52:A:N7 | 2.24 | 0.52 |
| 25:U:51:LEU:N | 25:U:53:GLN:NE2 | 2.58 | 0.52 |
| 2:B:286:U:H2' | 2:B:287:G:H8 | 1.71 | 0.52 |
| 13:3:60:CYS:C | 13:3:62:PRO:HD3 | 2.30 | 0.52 |
| 2:B:2700:A:H2' | 2:B:2701:U:H6 | 1.72 | 0.52 |
| 4:C:33:LEU:HD23 | 4:C:62:ARG:HA | 1.91 | 0.52 |
| 2:B:1573:G:H2' | 2:B:1574:C:H5' | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:159:G:O2' | 2:B:160:A:H5'' | 2.09 | 0.52 |
| 23:Q:56:PHE:O | 23:Q:59:LEU:HB3 | 2.10 | 0.52 |
| 19:H:4:ILE:HA | 19:H:18:GLN:HA | 1.91 | 0.52 |
| 19:H:31:VAL:HB | 19:H:32:PRO:HD3 | 1.84 | 0.52 |
| 2:B:547:A:H4' | 2:B:547:A:OP2 | 2.09 | 0.52 |
| 2:B:741:U:H2' | 2:B:742:A:C8 | 2.45 | 0.52 |
| 2:B:743:A:C2' | 2:B:744:U:H5' | 2.40 | 0.52 |
| 2:B:1439:A:C5 | 2:B:1552:A:N6 | 2.77 | 0.52 |
| 2:B:1021:A:H61 | 2:B:1142:A:N6 | 2.07 | 0.52 |
| 21:N:92:GLY:HA2 | 21:N:94:TYR:CZ | 2.45 | 0.52 |
| 25:U:10:VAL:HG21 | 25:U:35:VAL:HG22 | 1.91 | 0.52 |
| 8:E:117:ARG:HA | 8:E:185:LYS:NZ | 2.24 | 0.52 |
| 2:B:664:G:H4' | 2:B:941:A:OP1 | 2.09 | 0.52 |
| 13:3:21:PHE:CE1 | 13:3:58:ILE:HG12 | 2.44 | 0.52 |
| 2:B:947:A:H2' | 2:B:948:C:H6 | 1.72 | 0.52 |
| 20:J:64:VAL:O | 20:J:68:LYS:HD2 | 2.10 | 0.52 |
| 3:I:99:LYS:HD3 | 3:I:99:LYS:N | 2.24 | 0.52 |
| 2:B:2748:A:H1' | 27:G:66:THR:HB | 1.90 | 0.52 |
| 8:E:111:GLU:HG2 | 8:E:114:ARG:NH2 | 2.24 | 0.52 |
| 27:G:25:ILE:HD13 | 27:G:74:MET:HE2 | 1.89 | 0.52 |
| 11:4:2:LYS:HD3 | 11:4:4:ARG:HG3 | 1.90 | 0.52 |
| 24:S:66:ILE:H | 24:S:66:ILE:CD1 | 2.17 | 0.52 |
| 16:L:112:LEU:O | 16:L:112:LEU:HD23 | 2.09 | 0.52 |
| 27:G:94:ARG:NH2 | 27:G:104:LEU:HA | 2.23 | 0.52 |
| 2:B:1571:A:H2' | 2:B:1572:A:C8 | 2.44 | 0.52 |
| 20:J:59:ALA:C | 20:J:61:LYS:H | 2.13 | 0.52 |
| 2:B:812:C:H5' | 16:L:21:ARG:O | 2.09 | 0.52 |
| 4:C:34:GLU:O | 4:C:34:GLU:HG3 | 2.09 | 0.52 |
| 2:B:765:C:H2' | 2:B:766:U:C6 | 2.44 | 0.52 |
| 4:C:2:VAL:HG23 | 4:C:3:VAL:H | 1.74 | 0.52 |
| 2:B:1690:A:H2' | 2:B:1691:C:O4' | 2.10 | 0.52 |
| 6:K:109:SER:C | 6:K:111:LYS:H | 2.13 | 0.52 |
| 4:C:117:SER:HB3 | 4:C:128:THR:HB | 1.92 | 0.52 |
| 23:Q:97:ILE:HG13 | 23:Q:105:PHE:HB2 | 1.91 | 0.52 |
| 5:D:175:LEU:HD11 | 5:D:193:VAL:HG12 | 1.91 | 0.52 |
| 17:M:41:LEU:HD22 | 17:M:124:LEU:HD22 | 1.92 | 0.52 |
| 6:K:47:ILE:CG1 | 6:K:48:PRO:HD2 | 2.34 | 0.52 |
| 30:Z:68:LEU:HD22 | 30:Z:78:TYR:CD1 | 2.45 | 0.52 |
| 2:B:357:C:H2' | 2:B:358:U:C6 | 2.44 | 0.52 |
| 2:B:326:G:O2' | 2:B:327:G:H5' | 2.09 | 0.52 |
| 2:B:1590:A:H2' | 2:B:1591:A:C8 | 2.44 | 0.52 |
| 9:Y:2:LYS:HG2 | 9:Y:3:THR:H | 1.73 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 5:D:118:PHE:O | 5:D:119:ALA:HB3 | 2.10 | 0.52 |
| 21:N:97:ILE:HD12 | 21:N:98:LEU:H | 1.75 | 0.52 |
| 8:E:170:ARG:HH22 | 8:E:176:ASP:CB | 2.23 | 0.52 |
| 26:F:147:ARG:CZ | 26:F:147:ARG:HB3 | 2.39 | 0.52 |
| 2:B:1843:C:O2' | 2:B:1844:C:H5' | 2.09 | 0.52 |
| 2:B:1509:A:H3' | 2:B:1510:G:H5' | 1.91 | 0.52 |
| 14:V:80:HIS:CD2 | 14:V:82:TYR:H | 2.26 | 0.52 |
| 2:B:2106:U:H2' | 2:B:2107:G:C8 | 2.45 | 0.52 |
| 2:B:813:U:H2' | 2:B:814:C:H6 | 1.72 | 0.52 |
| 2:B:1557:C:H3' | 2:B:1558:C:H5'' | 1.91 | 0.52 |
| 2:B:2489:U:O2' | 2:B:2490:G:H5' | 2.09 | 0.52 |
| 2:B:1319:C:O2' | 2:B:1320:C:H5' | 2.10 | 0.52 |
| 2:B:738:G:H1' | 2:B:759:G:N2 | 2.24 | 0.52 |
| 23:Q:52:ARG:C | 23:Q:54:ARG:H | 2.13 | 0.52 |
| 19:H:18:GLN:HE21 | 19:H:39:ALA:CB | 2.20 | 0.52 |
| 5:D:11:MET:HE2 | 5:D:192:ALA:H | 1.73 | 0.52 |
| 19:H:88:GLY:O | 19:H:124:THR:HA | 2.10 | 0.52 |
| 7:P:54:LEU:HA | 7:P:76:HIS:HD2 | 1.74 | 0.52 |
| 2:B:2061:G:H5'' | 2:B:2503:A:C2 | 2.45 | 0.52 |
| 17:M:4:PRO:CG | 17:M:70:ASP:HA | 2.39 | 0.52 |
| 2:B:1083:U:H2' | 2:B:1085:A:OP2 | 2.10 | 0.52 |
| 19:H:72:ILE:HG12 | 19:H:108:VAL:HG11 | 1.90 | 0.52 |
| 2:B:1275:A:H2' | 2:B:1276:A:O4' | 2.10 | 0.52 |
| 2:B:414:C:H2' | 2:B:415:A:H8 | 1.74 | 0.52 |
| 4:C:216:ARG:HH11 | 4:C:216:ARG:HG3 | 1.75 | 0.52 |
| 2:B:516:C:O2' | 2:B:517:C:H5' | 2.09 | 0.52 |
| 2:B:1526:C:H2' | 2:B:1527:G:O4' | 2.09 | 0.52 |
| 7:P:31:VAL:O | 7:P:32:VAL:HB | 2.10 | 0.52 |
| 2:B:2336:A:H1' | 2:B:2337:G:OP1 | 2.09 | 0.52 |
| 16:L:93:ASN:O | 16:L:95:LEU:N | 2.42 | 0.52 |
| 5:D:55:LYS:HG3 | 5:D:60:VAL:HG13 | 1.90 | 0.52 |
| 2:B:1060:U:H5 | 3:I:131:THR:HG22 | 1.75 | 0.52 |
| 3:I:24:GLY:HA2 | 3:I:34:ILE:HD12 | 1.91 | 0.52 |
| 2:B:126:A:H5' | 15:2:19:ARG:HD2 | 1.92 | 0.52 |
| 2:B:851:C:H2' | 2:B:852:U:C6 | 2.45 | 0.52 |
| 12:1:24:LYS:HD3 | 12:1:52:LYS:HB2 | 1.90 | 0.52 |
| 25:U:12:VAL:HG21 | 25:U:38:ILE:HG12 | 1.91 | 0.52 |
| 13:3:31:ILE:HD11 | 13:3:34:LYS:CD | 2.37 | 0.52 |
| 2:B:2415:G:H4' | 16:L:66:PHE:HB2 | 1.91 | 0.52 |
| 2:B:2897:U:H2' | 2:B:2898:U:H6 | 1.75 | 0.52 |
| 2:B:1163:G:H4' | 28:R:92:TRP:CD1 | 2.45 | 0.52 |
| 2:B:825:A:O2' | 16:L:54:GLN:HB3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 17:M:111:GLU:HA | 17:M:114:ARG:HH22 | 1.73 | 0.52 |
| 2:B:2189:U:C2' | 2:B:2190:G:H5' | 2.39 | 0.52 |
| 13:3:44:ARG:N | 13:3:45:PRO:HD2 | 2.25 | 0.52 |
| 2:B:1683:U:H2' | 2:B:1684:G:C8 | 2.44 | 0.52 |
| 19:H:87:GLU:N | 19:H:87:GLU:CD | 2.63 | 0.52 |
| 5:D:46:ARG:NH1 | 5:D:85:ALA:HA | 2.24 | 0.52 |
| 19:H:42:LYS:O | 19:H:45:GLU:HB2 | 2.10 | 0.52 |
| 14:V:63:ILE:HD12 | 14:V:63:ILE:N | 2.25 | 0.52 |
| 2:B:1060:U:O2 | 2:B:1088:A:C8 | 2.63 | 0.52 |
| 5:D:149:ASN:H | 5:D:152:PRO:HG2 | 1.75 | 0.52 |
| 2:B:125:A:H4' | 2:B:126:A:OP2 | 2.10 | 0.52 |
| 11:4:17:VAL:HG12 | 11:4:18:LYS:N | 2.21 | 0.52 |
| 21:N:45:ARG:O | 21:N:49:GLU:HG3 | 2.09 | 0.52 |
| 8:E:109:LEU:HD13 | 8:E:180:LEU:HD13 | 1.92 | 0.52 |
| 14:V:62:THR:HA | 14:V:71:LYS:HA | 1.92 | 0.52 |
| 2:B:151:C:H2' | 2:B:152:A:C8 | 2.44 | 0.52 |
| 2:B:2210:U:N3 | 2:B:2212:A:N7 | 2.58 | 0.52 |
| 2:B:2636:C:H2' | 2:B:2637:U:C6 | 2.45 | 0.52 |
| 5:D:38:LYS:HD3 | 5:D:45:TYR:OH | 2.09 | 0.52 |
| 3:I:92:PRO:O | 3:I:93:ASN:HB2 | 2.10 | 0.52 |
| 2:B:2336:A:O2' | 2:B:2337:G:P | 2.69 | 0.51 |
| 23:Q:59:LEU:O | 23:Q:62:ALA:HB3 | 2.10 | 0.51 |
| 2:B:2875:C:H2' | 2:B:2876:G:H8 | 1.75 | 0.51 |
| 16:L:29:LYS:O | 16:L:31:GLY:N | 2.40 | 0.51 |
| 6:K:43:ILE:HG22 | 6:K:54:LYS:HA | 1.92 | 0.51 |
| 28:R:19:THR:HG22 | 28:R:97:LYS:HG3 | 1.92 | 0.51 |
| 2:B:483:A:H4' | 25:U:45:GLN:O | 2.10 | 0.51 |
| 2:B:455:C:N3 | 2:B:473:G:H5' | 2.25 | 0.51 |
| 20:J:72:LYS:HB2 | 20:J:89:PHE:H | 1.76 | 0.51 |
| 2:B:2100:G:H2' | 2:B:2101:A:H8 | 1.74 | 0.51 |
| 17:M:105:MET:HE3 | 17:M:105:MET:HA | 1.91 | 0.51 |
| 2:B:2784:U:H2' | 2:B:2785:C:H6 | 1.74 | 0.51 |
| 8:E:137:LYS:HE2 | 8:E:141:MET:SD | 2.49 | 0.51 |
| 2:B:696:G:O2' | 2:B:697:G:H5' | 2.10 | 0.51 |
| 8:E:4:VAL:C | 8:E:6:LYS:H | 2.14 | 0.51 |
| 16:L:135:ILE:HG12 | 16:L:140:GLY:HA3 | 1.92 | 0.51 |
| 27:G:83:THR:HA | 27:G:84:LYS:HZ3 | 1.74 | 0.51 |
| 24:S:36:LEU:CD2 | 24:S:36:LEU:H | 2.22 | 0.51 |
| 2:B:2884:U:H2' | 2:B:2885:G:C8 | 2.45 | 0.51 |
| 12:1:37:LYS:H | 12:1:48:TYR:HD2 | 1.57 | 0.51 |
| 9:Y:40:THR:HG22 | 9:Y:41:PRO:HD2 | 1.92 | 0.51 |
| 7:P:91:VAL:CG2 | 7:P:96:LEU:HD21 | 2.38 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:E:176:ASP:OD1 | 8:E:178:VAL:HG12 | 2.09 | 0.51 |
| 4:C:245:THR:OG1 | 4:C:249:VAL:HG23 | 2.11 | 0.51 |
| 2:B:878:A:C1' | 2:B:899:A:H62 | 2.23 | 0.51 |
| 20:J:20:ALA:HA | 20:J:23:LYS:HG3 | 1.92 | 0.51 |
| 2:B:320:A:H4' | 2:B:322:A:N7 | 2.25 | 0.51 |
| 2:B:1374:G:H2' | 2:B:1375:U:C6 | 2.45 | 0.51 |
| 2:B:132:G:H2' | 2:B:133:U:C6 | 2.45 | 0.51 |
| 3:I:102:ARG:HG3 | 3:I:141:ASP:HB2 | 1.92 | 0.51 |
| 2:B:396:G:C6 | 2:B:397:U:C4 | 2.98 | 0.51 |
| 2:B:1098:A:C4 | 3:I:3:LYS:O | 2.64 | 0.51 |
| 27:G:24:THR:C | 27:G:25:ILE:HD12 | 2.29 | 0.51 |
| 20:J:44:TYR:CE2 | 23:Q:59:LEU:HD11 | 2.45 | 0.51 |
| 1:A:78:A:OP2 | 14:V:14:LYS:HE3 | 2.11 | 0.51 |
| 24:S:74:ILE:HD12 | 24:S:104:THR:O | 2.10 | 0.51 |
| 6:K:19:VAL:HB | 6:K:41:ILE:HD11 | 1.92 | 0.51 |
| 20:J:123:LYS:O | 20:J:124:VAL:HG13 | 2.09 | 0.51 |
| 12:1:3:GLY:C | 12:1:5:ARG:H | 2.13 | 0.51 |
| 8:E:118:LEU:HA | 8:E:186:VAL:HG13 | 1.93 | 0.51 |
| 5:D:113:SER:HB2 | 5:D:168:GLU:O | 2.11 | 0.51 |
| 2:B:2757:A:N3 | 2:B:2757:A:H2' | 2.24 | 0.51 |
| 2:B:2834:G:H1' | 2:B:2883:A:H61 | 1.75 | 0.51 |
| 25:U:60:LYS:HE2 | 25:U:60:LYS:HA | 1.92 | 0.51 |
| 2:B:1771:C:H2' | 2:B:1772:A:H8 | 1.76 | 0.51 |
| 2:B:2135:A:H61 | 2:B:2156:G:C2' | 2.24 | 0.51 |
| 4:C:53:ILE:O | 4:C:53:ILE:HG23 | 2.10 | 0.51 |
| 2:B:776:G:H4' | 2:B:777:G:O5' | 2.11 | 0.51 |
| 2:B:1260:A:H2' | 2:B:1261:C:C6 | 2.45 | 0.51 |
| 2:B:1099:G:H3' | 3:I:2:LYS:HA | 1.91 | 0.51 |
| 27:G:51:PHE:CD2 | 27:G:68:ARG:HG2 | 2.45 | 0.51 |
| 27:G:137:LYS:O | 27:G:140:ILE:HG13 | 2.10 | 0.51 |
| 2:B:1201:U:H2' | 2:B:1202:G:H8 | 1.76 | 0.51 |
| 26:F:102:LEU:HA | 26:F:106:ALA:CB | 2.40 | 0.51 |
| 2:B:1439:A:N7 | 2:B:1440:U:C2 | 2.79 | 0.51 |
| 2:B:1870:C:H5' | 2:B:1871:A:C8 | 2.45 | 0.51 |
| 2:B:2898:U:H2' | 2:B:2899:A:H8 | 1.75 | 0.51 |
| 8:E:3:LEU:O | 8:E:11:ALA:HA | 2.11 | 0.51 |
| 2:B:2803:G:H2' | 2:B:2804:U:C6 | 2.45 | 0.51 |
| 18:X:10:SER:N | 18:X:60:LYS:HE2 | 2.25 | 0.51 |
| 7:P:89:GLY:HA2 | 7:P:112:ARG:N | 2.25 | 0.51 |
| 21:N:9:GLN:O | 21:N:11:ASN:N | 2.43 | 0.51 |
| 2:B:1241:A:H5' | 2:B:1241:A:N3 | 2.26 | 0.51 |
| 2:B:2458:G:H1' | 2:B:2460:U:O4 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:2306:C:C5 | 2:B:2307:G:H2' | 2.46 | 0.51 |
| 3:I:76:ALA:HA | 3:I:135:MET:SD | 2.50 | 0.51 |
| 8:E:40:ARG:NH2 | 8:E:92:HIS:HE2 | 2.08 | 0.51 |
| 24:S:58:ALA:HB1 | 24:S:69:LEU:HD21 | 1.92 | 0.51 |
| 2:B:2386:A:H2' | 2:B:2387:U:C6 | 2.45 | 0.51 |
| 20:J:128:ASN:C | 20:J:129:GLU:HG3 | 2.30 | 0.51 |
| 16:L:4:ASN:N | 16:L:4:ASN:ND2 | 2.58 | 0.51 |
| 17:M:21:ALA:CB | 17:M:100:LYS:HG2 | 2.41 | 0.51 |
| 2:B:1804:C:OP1 | 4:C:256:THR:HB | 2.11 | 0.51 |
| 2:B:847:U:H3 | 2:B:933:A:H62 | 1.59 | 0.51 |
| 2:B:2892:G:H5'' | 2:B:2894:G:H22 | 1.76 | 0.51 |
| 5:D:124:ARG:HA | 5:D:165:MET:HE3 | 1.92 | 0.51 |
| 2:B:523:C:O2' | 2:B:524:G:H5' | 2.10 | 0.51 |
| 2:B:374:A:H61 | 2:B:400:G:H1' | 1.74 | 0.51 |
| 2:B:909:A:H2' | 2:B:912:C:H5 | 1.76 | 0.51 |
| 2:B:2889:C:O2' | 2:B:2890:G:H5' | 2.10 | 0.51 |
| 22:O:105:ALA:C | 22:O:107:ALA:H | 2.13 | 0.51 |
| 2:B:1248:G:C2 | 23:Q:2:ARG:HD2 | 2.46 | 0.51 |
| 2:B:1997:C:OP2 | 5:D:129:THR:HB | 2.10 | 0.51 |
| 10:O:32:THR:OG1 | 10:O:50:GLY:HA2 | 2.10 | 0.51 |
| 22:O:36:TYR:CD2 | 22:O:36:TYR:N | 2.78 | 0.51 |
| 16:L:82:LEU:O | 16:L:85:VAL:HG12 | 2.10 | 0.51 |
| 23:Q:63:ARG:HH21 | 23:Q:64:ILE:HD13 | 1.76 | 0.51 |
| 4:C:171:VAL:HG23 | 4:C:185:ALA:HB2 | 1.92 | 0.51 |
| 2:B:79:C:O2' | 2:B:346:A:H1' | 2.10 | 0.51 |
| 26:F:133:GLU:HA | 26:F:150:GLY:HA2 | 1.92 | 0.51 |
| 4:C:91:ALA:CB | 4:C:105:ALA:HB2 | 2.40 | 0.51 |
| 3:I:57:VAL:HG23 | 3:I:71:LYS:NZ | 2.25 | 0.51 |
| 17:M:40:ARG:HB2 | 17:M:93:VAL:HG22 | 1.91 | 0.51 |
| 2:B:356:G:H2' | 2:B:357:C:C6 | 2.46 | 0.51 |
| 9:Y:47:ILE:HG23 | 9:Y:54:VAL:HG21 | 1.91 | 0.51 |
| 27:G:86:LEU:HD21 | 27:G:148:ARG:HB3 | 1.91 | 0.51 |
| 13:3:51:LYS:HD2 | 13:3:54:LEU:HD22 | 1.91 | 0.51 |
| 2:B:418:C:H2' | 2:B:419:U:C6 | 2.46 | 0.51 |
| 2:B:1737:G:H5' | 2:B:1738:G:OP2 | 2.11 | 0.51 |
| 8:E:195:GLN:HA | 8:E:198:GLU:OE1 | 2.09 | 0.51 |
| 2:B:1275:A:N6 | 2:B:1296:G:H4' | 2.26 | 0.51 |
| 2:B:962:G:H21 | 2:B:2250:G:H22 | 1.57 | 0.51 |
| 2:B:299:A:H2' | 2:B:300:A:C8 | 2.46 | 0.51 |
| 1:A:54:G:H21 | 26:F:25:MET:CE | 2.23 | 0.51 |
| 2:B:2365:G:H4' | 31:W:59:PHE:HD1 | 1.73 | 0.51 |
| 4:C:128:THR:HA | 4:C:190:THR:CA | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 27:G:34:ARG:H | 27:G:34:ARG:CD | 2.24 | 0.51 |
| 20:J:24:THR:OG1 | 20:J:27:ARG:HD2 | 2.11 | 0.51 |
| 5:D:61:THR:O | 5:D:64:GLU:HB2 | 2.11 | 0.51 |
| 23:Q:4:LYS:O | 23:Q:5:ARG:HB2 | 2.11 | 0.51 |
| 2:B:2303:G:H4' | 26:F:121:PHE:O | 2.10 | 0.51 |
| 2:B:1438:U:O2' | 2:B:1439:A:H5' | 2.09 | 0.51 |
| 2:B:2144:G:C2 | 2:B:2146:C:H5' | 2.45 | 0.51 |
| 2:B:1487:U:H2' | 2:B:1488:C:C6 | 2.45 | 0.51 |
| 18:X:50:VAL:HG12 | 18:X:54:LYS:HD2 | 1.92 | 0.51 |
| 2:B:981:A:H4' | 2:B:2037:A:H5' | 1.93 | 0.51 |
| 2:B:2394:C:O2' | 2:B:2395:C:H5' | 2.11 | 0.51 |
| 2:B:2748:A:H4' | 27:G:3:VAL:HG21 | 1.93 | 0.51 |
| 8:E:111:GLU:HG2 | 8:E:114:ARG:HH22 | 1.74 | 0.51 |
| 17:M:63:ILE:HD12 | 17:M:63:ILE:H | 1.75 | 0.51 |
| 4:C:202:ARG:NH1 | 4:C:213:ARG:HE | 2.08 | 0.51 |
| 2:B:2624:G:H1' | 10:0:18:HIS:CE1 | 2.46 | 0.51 |
| 2:B:2365:G:H4' | 31:W:59:PHE:CE1 | 2.45 | 0.51 |
| 31:W:39:GLN:CG | 31:W:40:ARG:N | 2.74 | 0.51 |
| 23:Q:7:VAL:HG23 | 23:Q:8:ILE:N | 2.26 | 0.51 |
| 29:T:59:ASN:O | 29:T:84:TYR:HB2 | 2.11 | 0.51 |
| 18:X:8:GLU:O | 18:X:12:GLU:HB2 | 2.10 | 0.51 |
| 2:B:280:U:H2' | 2:B:281:C:C5 | 2.46 | 0.51 |
| 1:A:43:C:H4' | 26:F:91:ARG:NE | 2.26 | 0.51 |
| 5:D:118:PHE:HE2 | 21:N:1:MET:SD | 2.34 | 0.51 |
| 2:B:1381:G:H1' | 2:B:1571:A:N1 | 2.26 | 0.51 |
| 2:B:2241:A:H2' | 2:B:2242:G:H8 | 1.76 | 0.51 |
| 18:X:14:LEU:O | 18:X:18:LEU:HB2 | 2.11 | 0.51 |
| 23:Q:57:ARG:HG2 | 23:Q:57:ARG:HH11 | 1.76 | 0.51 |
| 5:D:47:ALA:HB2 | 5:D:83:ARG:HD2 | 1.92 | 0.51 |
| 2:B:132:G:O2' | 2:B:133:U:H5' | 2.11 | 0.51 |
| 2:B:942:G:H2' | 2:B:943:A:H8 | 1.76 | 0.51 |
| 2:B:492:A:H2' | 2:B:493:G:O4' | 2.11 | 0.51 |
| 2:B:2247:A:H2' | 2:B:2248:C:C6 | 2.46 | 0.51 |
| 2:B:1038:G:O2' | 2:B:1039:A:H5' | 2.10 | 0.51 |
| 2:B:1266:G:N2 | 2:B:2012:G:H2' | 2.25 | 0.51 |
| 20:J:24:THR:O | 20:J:25:LEU:HB3 | 2.11 | 0.51 |
| 14:V:30:ILE:O | 14:V:37:PRO:HA | 2.10 | 0.51 |
| 5:D:8:LYS:HG2 | 5:D:197:THR:N | 2.24 | 0.51 |
| 24:S:51:LEU:C | 24:S:53:SER:H | 2.14 | 0.51 |
| 19:H:9:VAL:HG12 | 19:H:12:LEU:HG | 1.93 | 0.51 |
| 2:B:2529:G:O3' | 27:G:174:LYS:HE2 | 2.11 | 0.51 |
| 5:D:92:VAL:O | 5:D:94:GLN:N | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 22:O:39:VAL:HB | 22:O:49:VAL:HG22 | 1.93 | 0.51 |
| 2:B:506:G:H1' | 2:B:507:A:C8 | 2.46 | 0.51 |
| 30:Z:27:ARG:HD2 | 30:Z:29:PHE:CE1 | 2.46 | 0.51 |
| 28:R:78:ARG:HH21 | 28:R:78:ARG:HG3 | 1.76 | 0.51 |
| 2:B:2882:A:H3' | 2:B:2883:A:H5'' | 1.92 | 0.51 |
| 2:B:718:A:H3' | 2:B:719:C:C6 | 2.44 | 0.51 |
| 2:B:1430:G:H2' | 2:B:1431:A:C8 | 2.46 | 0.51 |
| 2:B:1430:G:H2' | 2:B:1431:A:H8 | 1.75 | 0.51 |
| 14:V:6:ALA:HB3 | 14:V:65:VAL:CG1 | 2.40 | 0.51 |
| 2:B:102:U:H2' | 18:X:2:LYS:CE | 2.41 | 0.51 |
| 2:B:1459:G:O2' | 2:B:1460:U:H5' | 2.11 | 0.51 |
| 2:B:1932:A:H2' | 2:B:1933:G:O4' | 2.11 | 0.51 |
| 20:J:45:THR:OG1 | 20:J:48:VAL:HB | 2.11 | 0.51 |
| 2:B:994:C:O2 | 28:R:10:LYS:HE3 | 2.11 | 0.51 |
| 29:T:27:SER:O | 29:T:28:ASN:HB3 | 2.11 | 0.51 |
| 5:D:9:VAL:O | 7:P:4:ILE:HD11 | 2.11 | 0.51 |
| 3:I:100:ILE:O | 3:I:139:VAL:HA | 2.11 | 0.51 |
| 8:E:146:VAL:HA | 8:E:185:LYS:O | 2.11 | 0.51 |
| 6:K:118:LEU:C | 6:K:120:PRO:HD2 | 2.30 | 0.51 |
| 2:B:533:G:H2' | 2:B:534:U:C6 | 2.46 | 0.51 |
| 15:2:26:ASN:HA | 15:2:29:GLN:HB3 | 1.93 | 0.51 |
| 5:D:33:ARG:NE | 5:D:74:GLU:HB3 | 2.26 | 0.51 |
| 2:B:1418:G:H1' | 2:B:1580:A:H61 | 1.75 | 0.51 |
| 2:B:1794:A:O2' | 2:B:1795:C:H5' | 2.11 | 0.51 |
| 2:B:2189:U:H2' | 2:B:2190:G:H5' | 1.93 | 0.51 |
| 2:B:2025:C:H2' | 2:B:2026:U:C6 | 2.46 | 0.51 |
| 8:E:130:LYS:C | 8:E:132:LYS:H | 2.14 | 0.51 |
| 2:B:1877:A:H2' | 2:B:1878:G:H8 | 1.75 | 0.51 |
| 4:C:209:ALA:HA | 4:C:212:TRP:NE1 | 2.26 | 0.51 |
| 17:M:90:GLU:OE1 | 17:M:90:GLU:HA | 2.11 | 0.51 |
| 7:P:83:ILE:HD13 | 7:P:83:ILE:O | 2.11 | 0.51 |
| 2:B:536:G:H21 | 20:J:47:HIS:CG | 2.29 | 0.51 |
| 2:B:98:G:H22 | 25:U:6:ARG:NH1 | 2.09 | 0.51 |
| 2:B:1341:G:H2' | 2:B:1397:U:O2' | 2.11 | 0.51 |
| 4:C:270:ARG:HG2 | 4:C:271:SER:N | 2.25 | 0.51 |
| 1:A:111:U:H2' | 1:A:112:G:C8 | 2.46 | 0.51 |
| 2:B:1099:G:OP2 | 3:I:2:LYS:O | 2.29 | 0.50 |
| 2:B:1099:G:C8 | 3:I:3:LYS:CB | 2.94 | 0.50 |
| 23:Q:111:LYS:HD2 | 28:R:50:GLY:HA3 | 1.92 | 0.50 |
| 28:R:16:GLU:HG2 | 28:R:101:ILE:HG13 | 1.93 | 0.50 |
| 3:I:79:LEU:HD11 | 3:I:131:THR:OG1 | 2.11 | 0.50 |
| 27:G:84:LYS:HB3 | 27:G:132:LEU:HG | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 31:W:37:VAL:CG1 | 31:W:38:ARG:HD3 | 2.42 | 0.50 |
| 2:B:2719:G:O2' | 2:B:2720:U:H5' | 2.11 | 0.50 |
| 2:B:1439:A:N7 | 2:B:1440:U:N1 | 2.59 | 0.50 |
| 2:B:1442:U:H2' | 2:B:1443:U:H6 | 1.76 | 0.50 |
| 2:B:143:C:H2' | 2:B:144:A:H8 | 1.75 | 0.50 |
| 25:U:9:GLU:O | 25:U:72:PHE:N | 2.44 | 0.50 |
| 2:B:2334:U:O3' | 22:O:13:ARG:HD3 | 2.12 | 0.50 |
| 2:B:2312:U:H5' | 26:F:84:ILE:HD12 | 1.93 | 0.50 |
| 20:J:64:VAL:HG13 | 20:J:68:LYS:HB2 | 1.93 | 0.50 |
| 2:B:2774:C:H2' | 2:B:2775:G:O4' | 2.11 | 0.50 |
| 1:A:60:C:H2' | 1:A:61:G:C8 | 2.46 | 0.50 |
| 2:B:1001:A:H2' | 2:B:1002:G:O4' | 2.11 | 0.50 |
| 2:B:1111:A:H4' | 2:B:1112:G:H4' | 1.93 | 0.50 |
| 2:B:2605:U:H2' | 2:B:2606:C:C6 | 2.46 | 0.50 |
| 2:B:2262:U:O2' | 2:B:2263:C:H5' | 2.11 | 0.50 |
| 2:B:2099:U:O2 | 2:B:2099:U:H2' | 2.10 | 0.50 |
| 2:B:660:C:H2' | 2:B:661:A:H8 | 1.76 | 0.50 |
| 31:W:70:VAL:HG23 | 31:W:75:ASN:ND2 | 2.25 | 0.50 |
| 26:F:37:MET:SD | 26:F:52:ALA:HB1 | 2.51 | 0.50 |
| 2:B:2470:G:P | 17:M:55:ARG:HH11 | 2.34 | 0.50 |
| 27:G:53:PRO:HG3 | 27:G:61:TRP:CD2 | 2.46 | 0.50 |
| 23:Q:107:ALA:HA | 23:Q:110:GLU:OE1 | 2.09 | 0.50 |
| 3:I:54:ILE:C | 3:I:54:ILE:HD13 | 2.30 | 0.50 |
| 26:F:102:LEU:HD22 | 26:F:103:ILE:H | 1.76 | 0.50 |
| 26:F:106:ALA:N | 26:F:108:PRO:HD2 | 2.26 | 0.50 |
| 26:F:135:ILE:CD1 | 26:F:137:PHE:HB3 | 2.33 | 0.50 |
| 2:B:1287:A:H3' | 2:B:1288:G:H21 | 1.75 | 0.50 |
| 2:B:1552:A:H2' | 2:B:1553:A:C5' | 2.40 | 0.50 |
| 8:E:58:LYS:HD3 | 8:E:58:LYS:N | 2.26 | 0.50 |
| 2:B:1285:A:H2' | 2:B:1286:A:H5'' | 1.92 | 0.50 |
| 16:L:3:LEU:HA | 16:L:6:LEU:HD21 | 1.94 | 0.50 |
| 1:A:32:U:H2' | 1:A:33:G:O4' | 2.11 | 0.50 |
| 9:Y:40:THR:O | 9:Y:43:ILE:HG22 | 2.11 | 0.50 |
| 5:D:69:ALA:N | 5:D:73:VAL:HB | 2.26 | 0.50 |
| 2:B:667:U:H2' | 2:B:668:A:O4' | 2.11 | 0.50 |
| 2:B:2038:G:H2' | 2:B:2039:U:O4' | 2.12 | 0.50 |
| 2:B:393:C:O2' | 2:B:394:C:H5' | 2.11 | 0.50 |
| 2:B:817:C:O2' | 2:B:839:U:H5'' | 2.11 | 0.50 |
| 5:D:169:ARG:O | 5:D:170:VAL:HG22 | 2.11 | 0.50 |
| 2:B:2341:G:H2' | 2:B:2342:C:C6 | 2.46 | 0.50 |
| 27:G:154:GLU:HG2 | 27:G:154:GLU:O | 2.10 | 0.50 |
| 2:B:1460:U:H5'' | 2:B:1461:C:O4' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:O:28:VAL:HG21 | 22:O:106:LEU:HD21 | 1.93 | 0.50 |
| 4:C:202:ARG:CB | 4:C:202:ARG:HH21 | 2.23 | 0.50 |
| 2:B:2411:A:H2' | 2:B:2412:A:C8 | 2.46 | 0.50 |
| 2:B:497:A:H2' | 2:B:498:G:O4' | 2.11 | 0.50 |
| 2:B:2512:C:H2' | 2:B:2513:A:O4' | 2.12 | 0.50 |
| 8:E:106:LYS:HE3 | 8:E:200:LEU:HB3 | 1.92 | 0.50 |
| 2:B:2376:A:N1 | 22:O:92:PHE:HD2 | 2.10 | 0.50 |
| 2:B:2836:U:H2' | 2:B:2837:A:C8 | 2.46 | 0.50 |
| 10:O:25:THR:O | 10:O:26:SER:HB3 | 2.11 | 0.50 |
| 2:B:1642:G:O2' | 2:B:1643:G:H5' | 2.11 | 0.50 |
| 5:D:204:LYS:HB2 | 5:D:205:PRO:HD2 | 1.91 | 0.50 |
| 16:L:124:GLY:O | 16:L:125:LEU:HG | 2.12 | 0.50 |
| 27:G:17:LYS:CA | 27:G:17:LYS:HZ2 | 2.24 | 0.50 |
| 20:J:25:LEU:HD13 | 20:J:26:GLY:N | 2.26 | 0.50 |
| 5:D:178:VAL:HG12 | 5:D:179:ARG:HG3 | 1.92 | 0.50 |
| 3:I:78:LEU:HD13 | 3:I:108:ILE:HG23 | 1.94 | 0.50 |
| 23:Q:65:ASN:O | 23:Q:69:ARG:HB2 | 2.11 | 0.50 |
| 5:D:68:PHE:C | 5:D:73:VAL:HB | 2.31 | 0.50 |
| 2:B:947:A:O2' | 2:B:984:A:H2 | 1.94 | 0.50 |
| 2:B:1411:U:H2' | 2:B:1412:U:C6 | 2.46 | 0.50 |
| 2:B:1507:C:C2' | 2:B:1508:A:H4' | 2.41 | 0.50 |
| 31:W:47:GLY:HA3 | 31:W:80:SER:CB | 2.41 | 0.50 |
| 2:B:864:G:O2' | 2:B:865:C:H5' | 2.11 | 0.50 |
| 6:K:3:GLN:HG2 | 6:K:4:GLU:N | 2.27 | 0.50 |
| 2:B:1824:G:O2' | 2:B:1825:U:H5' | 2.10 | 0.50 |
| 29:T:5:GLU:HA | 29:T:8:LEU:HD12 | 1.93 | 0.50 |
| 16:L:92:LEU:HD21 | 16:L:123:ARG:NH2 | 2.25 | 0.50 |
| 14:V:77:VAL:HG11 | 17:M:136:MET:HB3 | 1.93 | 0.50 |
| 7:P:5:LYS:O | 7:P:9:GLN:HG2 | 2.10 | 0.50 |
| 27:G:116:LEU:HD23 | 27:G:120:ILE:CD1 | 2.40 | 0.50 |
| 8:E:33:VAL:O | 8:E:36:ALA:HB3 | 2.11 | 0.50 |
| 2:B:1454:C:H5' | 21:N:63:ARG:NE | 2.26 | 0.50 |
| 21:N:83:LEU:HA | 21:N:86:ARG:CG | 2.35 | 0.50 |
| 31:W:37:VAL:C | 31:W:38:ARG:HG2 | 2.31 | 0.50 |
| 2:B:2720:U:H5'' | 7:P:52:ARG:HH21 | 1.74 | 0.50 |
| 15:2:42:LEU:O | 15:2:43:THR:HG23 | 2.11 | 0.50 |
| 30:Z:7:VAL:HG21 | 30:Z:59:ILE:CD1 | 2.39 | 0.50 |
| 2:B:1654:A:H2' | 2:B:1655:A:C8 | 2.46 | 0.50 |
| 28:R:63:VAL:HA | 28:R:95:ASP:O | 2.12 | 0.50 |
| 2:B:1487:U:H2' | 2:B:1488:C:H6 | 1.76 | 0.50 |
| 2:B:636:G:H3' | 16:L:128:THR:CG2 | 2.40 | 0.50 |
| 2:B:246:C:H2' | 2:B:247:G:H5' | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 30:Z:15:GLY:O | 30:Z:27:ARG:HG3 | 2.10 | 0.50 |
| 1:A:29:A:H3' | 1:A:30:C:C6 | 2.44 | 0.50 |
| 2:B:2471:A:O2' | 2:B:2472:G:O5' | 2.30 | 0.50 |
| 2:B:632:A:H2' | 2:B:633:A:C8 | 2.46 | 0.50 |
| 1:A:48:U:H2' | 1:A:49:C:C6 | 2.47 | 0.50 |
| 2:B:1828:G:O6 | 4:C:220:ARG:HD2 | 2.12 | 0.50 |
| 2:B:1275:A:N3 | 2:B:1275:A:H2' | 2.26 | 0.50 |
| 2:B:2095:A:H3' | 2:B:2096:C:H6 | 1.75 | 0.50 |
| 6:K:53:LYS:HD3 | 6:K:56:ASP:OD2 | 2.12 | 0.50 |
| 8:E:1:MET:HB3 | 8:E:14:VAL:O | 2.12 | 0.50 |
| 4:C:73:ILE:HG21 | 4:C:97:ASP:HB2 | 1.92 | 0.50 |
| 2:B:572:A:H5'' | 28:R:80:ARG:NH2 | 2.26 | 0.50 |
| 8:E:5:LEU:HD13 | 8:E:122:GLU:HG3 | 1.94 | 0.50 |
| 26:F:72:SER:OG | 26:F:79:ARG:HA | 2.11 | 0.50 |
| 2:B:1911:U:O2' | 2:B:1912:A:H5' | 2.12 | 0.50 |
| 8:E:58:LYS:HE2 | 8:E:60:TRP:CD1 | 2.45 | 0.50 |
| 2:B:137:U:H2' | 2:B:138:U:C6 | 2.46 | 0.50 |
| 9:Y:50:VAL:O | 9:Y:54:VAL:HG22 | 2.12 | 0.50 |
| 4:C:78:GLU:OE1 | 4:C:94:LEU:HD22 | 2.11 | 0.50 |
| 2:B:2415:G:H4' | 16:L:65:GLY:O | 2.12 | 0.50 |
| 22:O:88:LYS:HE3 | 22:O:114:GLY:O | 2.12 | 0.50 |
| 4:C:244:VAL:HB | 4:C:249:VAL:N | 2.26 | 0.50 |
| 4:C:16:VAL:N | 4:C:203:VAL:HG12 | 2.26 | 0.50 |
| 1:A:102:G:O2' | 1:A:103:U:H5' | 2.12 | 0.50 |
| 2:B:729:G:C5 | 4:C:206:LYS:HB2 | 2.46 | 0.50 |
| 2:B:418:C:H2' | 2:B:419:U:H6 | 1.76 | 0.50 |
| 2:B:1510:G:H2' | 2:B:1511:G:O4' | 2.11 | 0.50 |
| 2:B:1033:U:H5 | 11:4:15:LYS:HE3 | 1.76 | 0.50 |
| 22:O:100:HIS:C | 22:O:104:GLN:HB2 | 2.32 | 0.50 |
| 2:B:1219:U:H2' | 2:B:1220:G:C8 | 2.47 | 0.50 |
| 2:B:2257:U:O2' | 2:B:2258:C:H5' | 2.12 | 0.50 |
| 4:C:74:PRO:HG2 | 4:C:96:LYS:CG | 2.41 | 0.50 |
| 6:K:58:LEU:HD23 | 6:K:58:LEU:N | 2.26 | 0.50 |
| 27:G:103:ASN:HA | 27:G:113:ASP:HA | 1.93 | 0.50 |
| 2:B:1099:G:H5'' | 3:I:2:LYS:HB2 | 1.94 | 0.50 |
| 2:B:2273:A:H2' | 2:B:2274:A:C8 | 2.46 | 0.50 |
| 2:B:557:C:H2' | 2:B:558:U:H6 | 1.77 | 0.50 |
| 23:Q:55:GLN:O | 23:Q:59:LEU:HB2 | 2.11 | 0.50 |
| 17:M:68:PHE:CG | 17:M:69:PRO:HD2 | 2.47 | 0.50 |
| 26:F:3:LEU:HB2 | 26:F:100:GLU:OE2 | 2.11 | 0.50 |
| 2:B:544:C:O5' | 2:B:545:U:OP1 | 2.30 | 0.50 |
| 30:Z:5:CYS:CB | 30:Z:10:LYS:H | 2.22 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:117:G:H5' | 2:B:126:A:C8 | 2.41 | 0.50 |
| 25:U:93:ARG:O | 25:U:102:ILE:HG22 | 2.11 | 0.50 |
| 12:1:28:THR:O | 12:1:29:LYS:HD2 | 2.11 | 0.50 |
| 21:N:25:ALA:HA | 21:N:44:LEU:HD11 | 1.94 | 0.50 |
| 28:R:14:VAL:HG22 | 28:R:15:SER:N | 2.27 | 0.50 |
| 13:3:14:LYS:O | 13:3:21:PHE:O | 2.29 | 0.50 |
| 2:B:1506:U:H2' | 2:B:1507:C:C6 | 2.47 | 0.50 |
| 2:B:1734:G:O2' | 2:B:1735:A:H5' | 2.12 | 0.50 |
| 2:B:1159:U:O2' | 2:B:1160:G:H5' | 2.12 | 0.50 |
| 18:X:28:LEU:HD11 | 18:X:42:LEU:HD23 | 1.94 | 0.50 |
| 23:Q:104:ALA:O | 23:Q:105:PHE:HB3 | 2.11 | 0.50 |
| 4:C:43:ASN:HB2 | 4:C:49:THR:HG23 | 1.93 | 0.50 |
| 5:D:11:MET:H | 5:D:25:THR:HA | 1.75 | 0.50 |
| 2:B:2384:U:H5'' | 2:B:2386:A:OP1 | 2.12 | 0.50 |
| 31:W:35:ILE:O | 31:W:37:VAL:N | 2.45 | 0.50 |
| 5:D:34:VAL:HG12 | 5:D:94:GLN:H | 1.75 | 0.50 |
| 9:Y:6:ILE:HG22 | 9:Y:56:VAL:HA | 1.92 | 0.50 |
| 19:H:132:PHE:CD2 | 19:H:134:VAL:HG22 | 2.46 | 0.50 |
| 8:E:48:THR:H | 8:E:51:GLU:HG3 | 1.77 | 0.50 |
| 2:B:2213:U:O2' | 2:B:2214:C:H5' | 2.11 | 0.50 |
| 2:B:1355:G:O2' | 2:B:1356:G:H5' | 2.10 | 0.50 |
| 13:3:7:ARG:O | 13:3:11:LYS:HG3 | 2.12 | 0.50 |
| 26:F:115:GLY:HA3 | 26:F:177:ARG:HD2 | 1.93 | 0.50 |
| 5:D:154:LYS:HD3 | 5:D:154:LYS:N | 2.26 | 0.50 |
| 20:J:20:ALA:HA | 20:J:23:LYS:CG | 2.42 | 0.50 |
| 2:B:5:A:H2' | 2:B:6:A:H8 | 1.75 | 0.50 |
| 2:B:1260:A:H2' | 2:B:1261:C:H6 | 1.77 | 0.50 |
| 22:O:36:TYR:HD2 | 22:O:36:TYR:N | 2.09 | 0.50 |
| 2:B:1220:G:H2' | 2:B:1221:C:H6 | 1.76 | 0.50 |
| 2:B:2514:U:H2' | 2:B:2515:C:C6 | 2.47 | 0.50 |
| 2:B:758:C:O2 | 2:B:1981:A:H2 | 1.94 | 0.50 |
| 2:B:1098:A:H3' | 3:I:3:LYS:HB3 | 1.93 | 0.50 |
| 4:C:140:VAL:O | 4:C:141:HIS:HB2 | 2.12 | 0.50 |
| 23:Q:91:ARG:HE | 23:Q:94:LEU:CD2 | 2.23 | 0.50 |
| 26:F:110:ILE:HA | 26:F:111:ARG:NH1 | 2.26 | 0.50 |
| 26:F:12:VAL:O | 26:F:16:MET:HG2 | 2.11 | 0.50 |
| 7:P:47:ILE:HD11 | 7:P:59:THR:HG22 | 1.94 | 0.50 |
| 2:B:2037:A:H2' | 2:B:2038:G:H8 | 1.77 | 0.50 |
| 16:L:55:MET:HA | 16:L:55:MET:HE3 | 1.94 | 0.50 |
| 5:D:159:LYS:HZ2 | 5:D:160:LYS:N | 2.09 | 0.50 |
| 2:B:1373:A:H4' | 2:B:2212:A:N3 | 2.26 | 0.50 |
| 2:B:765:C:H2' | 2:B:766:U:H6 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2092:U:H4' | 2:B:2093:G:H5'' | 1.93 | 0.50 |
| 2:B:1396:U:O4' | 2:B:1396:U:O2 | 2.28 | 0.50 |
| 2:B:1858:A:C2 | 2:B:1859:U:H1' | 2.47 | 0.50 |
| 2:B:425:G:O2' | 2:B:426:C:H5' | 2.12 | 0.50 |
| 2:B:612:G:H2' | 2:B:614:A:H5'' | 1.94 | 0.50 |
| 4:C:259:ASN:C | 4:C:261:ARG:H | 2.15 | 0.50 |
| 2:B:1224:U:H4' | 28:R:88:GLY:O | 2.10 | 0.50 |
| 21:N:29:VAL:HG13 | 21:N:78:LYS:HG2 | 1.92 | 0.50 |
| 21:N:72:ASP:O | 21:N:76:VAL:HG13 | 2.11 | 0.50 |
| 24:S:71:VAL:O | 24:S:71:VAL:HG22 | 2.11 | 0.50 |
| 2:B:2314:A:C1' | 26:F:154:THR:HG21 | 2.39 | 0.50 |
| 2:B:2328:A:H2' | 2:B:2329:U:H6 | 1.75 | 0.50 |
| 2:B:2385:C:H2' | 2:B:2386:A:H8 | 1.75 | 0.50 |
| 2:B:126:A:H5' | 15:2:19:ARG:CD | 2.42 | 0.50 |
| 3:I:18:ASN:HB2 | 3:I:38:CYS:SG | 2.52 | 0.50 |
| 19:H:109:GLU:OE2 | 19:H:111:ALA:HB2 | 2.11 | 0.50 |
| 25:U:21:ARG:HD3 | 25:U:72:PHE:CD2 | 2.47 | 0.50 |
| 17:M:59:ARG:HE | 17:M:60:GLN:HB3 | 1.77 | 0.50 |
| 27:G:89:VAL:HG12 | 27:G:90:GLY:N | 2.24 | 0.50 |
| 18:X:46:VAL:O | 18:X:49:ASP:HB2 | 2.12 | 0.50 |
| 1:A:28:C:OP1 | 22:O:31:THR:HG21 | 2.12 | 0.50 |
| 2:B:2109:U:N3 | 2:B:2180:U:H2' | 2.26 | 0.50 |
| 2:B:264:C:C2' | 2:B:265:A:H5'' | 2.42 | 0.50 |
| 2:B:1028:A:N6 | 2:B:1125:G:H2' | 2.27 | 0.50 |
| 2:B:1434:A:H62 | 2:B:1558:C:H42 | 1.60 | 0.50 |
| 2:B:2783:U:H2' | 2:B:2784:U:C6 | 2.46 | 0.50 |
| 23:Q:57:ARG:HH12 | 23:Q:61:ILE:HD11 | 1.77 | 0.50 |
| 2:B:39:G:H2' | 2:B:40:U:H6 | 1.77 | 0.50 |
| 5:D:38:LYS:HD2 | 5:D:81:GLU:OE1 | 2.12 | 0.50 |
| 2:B:132:G:H2' | 2:B:133:U:H6 | 1.76 | 0.50 |
| 25:U:13:LEU:H | 25:U:13:LEU:HD12 | 1.77 | 0.50 |
| 2:B:1647:U:P | 2:B:1647:U:H3' | 2.52 | 0.50 |
| 1:A:85:G:H2' | 1:A:86:G:H8 | 1.77 | 0.50 |
| 2:B:2639:A:H2' | 2:B:2640:G:O4' | 2.11 | 0.50 |
| 2:B:2698:U:H2' | 2:B:2699:C:C6 | 2.47 | 0.50 |
| 27:G:39:ALA:HB1 | 27:G:57:TYR:CD1 | 2.46 | 0.50 |
| 31:W:50:VAL:CG2 | 31:W:61:LYS:HD3 | 2.35 | 0.49 |
| 4:C:130:PRO:HA | 4:C:188:ARG:HA | 1.94 | 0.49 |
| 5:D:25:THR:HG21 | 5:D:193:VAL:CG2 | 2.42 | 0.49 |
| 29:T:39:THR:HG22 | 29:T:42:GLU:CG | 2.42 | 0.49 |
| 4:C:80:LEU:HD23 | 4:C:91:ALA:HB2 | 1.93 | 0.49 |
| 21:N:55:ALA:HA | 21:N:80:PHE:CE1 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 31:W:37:VAL:HG11 | 31:W:38:ARG:HH11 | 1.76 | 0.49 |
| 6:K:43:ILE:CD1 | 6:K:52:VAL:HB | 2.42 | 0.49 |
| 27:G:153:PRO:CG | 27:G:162:ARG:HB3 | 2.42 | 0.49 |
| 8:E:161:ALA:HA | 8:E:164:LEU:HD12 | 1.94 | 0.49 |
| 2:B:1654:A:O2' | 5:D:118:PHE:CB | 2.60 | 0.49 |
| 2:B:616:A:H3' | 2:B:617:G:C8 | 2.42 | 0.49 |
| 2:B:592:A:C2 | 13:3:3:ILE:HD11 | 2.46 | 0.49 |
| 2:B:979:A:H2' | 2:B:982:C:H42 | 1.76 | 0.49 |
| 2:B:1409:U:H2' | 2:B:1410:G:C8 | 2.46 | 0.49 |
| 2:B:1199:U:H2' | 2:B:1200:C:H6 | 1.76 | 0.49 |
| 2:B:871:U:H2' | 2:B:872:U:C6 | 2.47 | 0.49 |
| 4:C:4:LYS:HE2 | 4:C:5:CYS:N | 2.27 | 0.49 |
| 2:B:2784:U:O2' | 2:B:2785:C:H5' | 2.12 | 0.49 |
| 2:B:753:A:H2' | 2:B:754:U:C6 | 2.47 | 0.49 |
| 2:B:1220:G:H2' | 2:B:1221:C:C6 | 2.46 | 0.49 |
| 4:C:74:PRO:HG2 | 4:C:96:LYS:HG2 | 1.94 | 0.49 |
| 2:B:2825:G:H5'' | 2:B:2825:G:N3 | 2.26 | 0.49 |
| 2:B:2199:A:H3' | 2:B:2200:C:H6 | 1.76 | 0.49 |
| 2:B:1564:C:H2' | 2:B:1565:C:C6 | 2.47 | 0.49 |
| 2:B:858:G:H21 | 2:B:2268:A:C3' | 2.24 | 0.49 |
| 16:L:95:LEU:HB3 | 16:L:100:ILE:HG23 | 1.93 | 0.49 |
| 27:G:24:THR:HB | 27:G:34:ARG:HD3 | 1.93 | 0.49 |
| 27:G:9:VAL:C | 27:G:11:PRO:HD3 | 2.31 | 0.49 |
| 27:G:96:ALA:O | 27:G:97:VAL:HB | 2.12 | 0.49 |
| 2:B:1245:G:H4' | 8:E:33:VAL:HG13 | 1.94 | 0.49 |
| 26:F:169:LEU:HB3 | 26:F:174:PHE:CD1 | 2.47 | 0.49 |
| 26:F:62:GLN:HE21 | 26:F:91:ARG:CZ | 2.25 | 0.49 |
| 2:B:677:A:O2' | 2:B:2071:A:H5' | 2.11 | 0.49 |
| 8:E:138:LEU:O | 8:E:142:ALA:N | 2.45 | 0.49 |
| 18:X:7:ARG:HH21 | 18:X:9:LYS:HD2 | 1.76 | 0.49 |
| 22:O:89:ASP:HA | 22:O:116:GLN:O | 2.11 | 0.49 |
| 20:J:96:ARG:N | 20:J:97:PRO:HD3 | 2.27 | 0.49 |
| 1:A:29:A:OP2 | 22:O:32:PRO:HD2 | 2.12 | 0.49 |
| 21:N:87:PHE:HE1 | 21:N:116:VAL:HG12 | 1.77 | 0.49 |
| 2:B:1418:G:H1' | 2:B:1580:A:N6 | 2.27 | 0.49 |
| 2:B:416:U:H2' | 2:B:417:C:H6 | 1.75 | 0.49 |
| 2:B:401:A:H2' | 2:B:402:A:C8 | 2.48 | 0.49 |
| 2:B:207:A:H2' | 2:B:208:C:O4' | 2.12 | 0.49 |
| 22:O:6:ALA:CB | 22:O:10:ARG:HH11 | 2.24 | 0.49 |
| 2:B:319:G:H2' | 2:B:320:A:O4' | 2.12 | 0.49 |
| 2:B:587:C:N3 | 16:L:33:ARG:NH2 | 2.60 | 0.49 |
| 2:B:1779:U:C5 | 2:B:1784:A:N7 | 2.80 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 9:Y:11:SER:OG | 9:Y:13:ILE:HG13 | 2.12 | 0.49 |
| 6:K:24:VAL:HG13 | 6:K:33:ALA:HB2 | 1.94 | 0.49 |
| 2:B:1390:U:O2' | 2:B:1391:U:H5' | 2.11 | 0.49 |
| 2:B:1092:C:H2' | 2:B:1093:G:H5' | 1.94 | 0.49 |
| 20:J:36:LEU:O | 20:J:51:GLY:HA3 | 2.13 | 0.49 |
| 5:D:32:ASN:HA | 5:D:51:THR:O | 2.12 | 0.49 |
| 26:F:107:VAL:HA | 26:F:111:ARG:HH12 | 1.76 | 0.49 |
| 8:E:61:ARG:O | 8:E:62:GLN:C | 2.50 | 0.49 |
| 2:B:359:G:H2' | 2:B:360:U:C5' | 2.38 | 0.49 |
| 3:I:21:PRO:CB | 3:I:22:PRO:HD3 | 2.38 | 0.49 |
| 2:B:141:G:O6 | 29:T:2:ILE:HG21 | 2.12 | 0.49 |
| 2:B:2728:U:H5' | 6:K:70:ARG:NH2 | 2.28 | 0.49 |
| 2:B:2592:G:H2' | 2:B:2593:U:O4' | 2.12 | 0.49 |
| 2:B:819:A:H5' | 2:B:973:A:N1 | 2.26 | 0.49 |
| 6:K:68:GLY:HA3 | 6:K:78:ARG:HB3 | 1.93 | 0.49 |
| 8:E:108:ILE:HD11 | 8:E:181:ILE:HB | 1.94 | 0.49 |
| 21:N:106:ASP:C | 21:N:108:ALA:H | 2.16 | 0.49 |
| 2:B:494:G:OP1 | 24:S:8:ARG:HD3 | 2.12 | 0.49 |
| 2:B:2825:G:H2' | 2:B:2826:A:H5' | 1.92 | 0.49 |
| 2:B:599:A:O2' | 2:B:600:G:H5' | 2.12 | 0.49 |
| 2:B:1816:C:H3' | 4:C:61:TYR:CE2 | 2.47 | 0.49 |
| 4:C:153:LEU:HD13 | 4:C:175:LEU:HD21 | 1.94 | 0.49 |
| 18:X:28:LEU:HB3 | 18:X:43:LEU:HD21 | 1.95 | 0.49 |
| 20:J:4:PHE:HB3 | 20:J:44:TYR:CD1 | 2.47 | 0.49 |
| 23:Q:73:ILE:HG21 | 23:Q:109:VAL:HG13 | 1.93 | 0.49 |
| 26:F:78:ILE:HA | 26:F:82:TYR:CG | 2.46 | 0.49 |
| 4:C:80:LEU:HD11 | 4:C:109:LEU:HG | 1.93 | 0.49 |
| 26:F:2:LYS:HD2 | 26:F:100:GLU:HG2 | 1.94 | 0.49 |
| 35:B:3741:HOH:O | 8:E:63:LYS:HE2 | 2.12 | 0.49 |
| 2:B:1141:U:H4' | 2:B:1142:A:C1' | 2.42 | 0.49 |
| 3:I:19:PRO:HB2 | 3:I:22:PRO:HD2 | 1.95 | 0.49 |
| 25:U:21:ARG:HG3 | 25:U:21:ARG:HH11 | 1.77 | 0.49 |
| 2:B:182:A:H2' | 2:B:183:C:C6 | 2.47 | 0.49 |
| 2:B:1785:A:O2' | 2:B:1786:A:H2' | 2.13 | 0.49 |
| 16:L:56:PRO:O | 16:L:59:ARG:HB2 | 2.12 | 0.49 |
| 2:B:526:A:N6 | 2:B:2626:C:C4' | 2.75 | 0.49 |
| 2:B:1403:A:H2' | 2:B:1404:C:C6 | 2.46 | 0.49 |
| 19:H:99:ILE:O | 19:H:103:VAL:HG12 | 2.13 | 0.49 |
| 2:B:2868:A:H2' | 2:B:2869:G:C8 | 2.47 | 0.49 |
| 3:I:2:LYS:C | 3:I:3:LYS:HD2 | 2.32 | 0.49 |
| 5:D:105:LYS:H | 5:D:106:LYS:NZ | 2.10 | 0.49 |
| 16:L:75:ALA:HB3 | 16:L:108:ALA:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:L:93:ASN:HA | 16:L:96:LYS:HD3 | 1.94 | 0.49 |
| 20:J:3:THR:HG21 | 23:Q:60:TRP:NE1 | 2.28 | 0.49 |
| 5:D:51:THR:HG22 | 5:D:52:THR:N | 2.28 | 0.49 |
| 29:T:74:ILE:HG13 | 29:T:75:GLY:N | 2.24 | 0.49 |
| 24:S:58:ALA:CB | 24:S:69:LEU:HD21 | 2.43 | 0.49 |
| 17:M:41:LEU:HD13 | 17:M:46:ILE:HG22 | 1.95 | 0.49 |
| 9:Y:2:LYS:HE2 | 9:Y:4:ILE:CD1 | 2.39 | 0.49 |
| 14:V:9:ARG:HA | 14:V:41:GLU:OE2 | 2.13 | 0.49 |
| 10:O:38:LEU:HB3 | 10:O:41:HIS:CD2 | 2.48 | 0.49 |
| 2:B:288:U:H2' | 2:B:289:G:C8 | 2.48 | 0.49 |
| 2:B:1299:G:H5'' | 2:B:1300:G:OP1 | 2.13 | 0.49 |
| 2:B:1031:G:H4' | 11:4:6:SER:HB3 | 1.94 | 0.49 |
| 2:B:309:A:N3 | 2:B:329:G:O2' | 2.45 | 0.49 |
| 2:B:1735:A:H2' | 2:B:1736:U:C6 | 2.47 | 0.49 |
| 2:B:702:U:H2' | 2:B:703:U:H6 | 1.76 | 0.49 |
| 23:Q:9:ALA:O | 23:Q:11:ALA:N | 2.45 | 0.49 |
| 28:R:54:VAL:HG13 | 28:R:56:GLY:O | 2.13 | 0.49 |
| 2:B:2636:C:H4' | 5:D:81:GLU:OE2 | 2.12 | 0.49 |
| 16:L:9:ALA:HB3 | 16:L:12:SER:OG | 2.12 | 0.49 |
| 2:B:1868:C:H2' | 2:B:1869:G:O4' | 2.12 | 0.49 |
| 2:B:690:G:H2' | 2:B:691:C:O4' | 2.12 | 0.49 |
| 27:G:15:ASP:HB2 | 27:G:26:LYS:HB3 | 1.94 | 0.49 |
| 23:Q:93:ILE:HG23 | 23:Q:94:LEU:H | 1.76 | 0.49 |
| 4:C:45:ASN:HB2 | 4:C:47:ARG:HG2 | 1.94 | 0.49 |
| 5:D:24:VAL:HA | 5:D:191:GLY:N | 2.27 | 0.49 |
| 14:V:79:ARG:NH1 | 17:M:134:THR:HG21 | 2.28 | 0.49 |
| 14:V:26:PHE:HE2 | 14:V:44:HIS:HA | 1.76 | 0.49 |
| 2:B:350:G:H2' | 2:B:351:C:O4' | 2.13 | 0.49 |
| 26:F:163:GLU:HA | 26:F:166:ARG:NH1 | 2.27 | 0.49 |
| 2:B:1551:A:H2' | 2:B:1552:A:O4' | 2.13 | 0.49 |
| 19:H:132:PHE:O | 19:H:139:PHE:HA | 2.11 | 0.49 |
| 2:B:2418:A:H2' | 2:B:2419:U:O4' | 2.12 | 0.49 |
| 6:K:99:ILE:N | 6:K:118:LEU:HD22 | 2.26 | 0.49 |
| 3:I:85:ILE:HD12 | 3:I:87:SER:O | 2.12 | 0.49 |
| 13:3:49:VAL:O | 13:3:51:LYS:N | 2.46 | 0.49 |
| 2:B:1515:A:H4' | 2:B:1556:C:O2' | 2.13 | 0.49 |
| 2:B:699:A:H4' | 2:B:1634:A:C5 | 2.48 | 0.49 |
| 27:G:154:GLU:C | 27:G:156:TYR:H | 2.16 | 0.49 |
| 18:X:23:ARG:O | 18:X:27:ASN:N | 2.46 | 0.49 |
| 2:B:95:A:H4' | 18:X:38:GLN:O | 2.12 | 0.49 |
| 2:B:1657:U:O2' | 2:B:1658:C:H5' | 2.11 | 0.49 |
| 2:B:2776:A:H4' | 2:B:2777:G:C5' | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:1036:G:H2' | 2:B:1037:G:H8 | 1.77 | 0.49 |
| 2:B:2098:U:H2' | 2:B:2099:U:C1' | 2.42 | 0.49 |
| 2:B:1564:C:O2' | 2:B:1565:C:H5' | 2.13 | 0.49 |
| 12:1:38:PHE:HB2 | 12:1:45:HIS:CE1 | 2.48 | 0.49 |
| 20:J:109:LEU:CD1 | 20:J:119:PHE:HB2 | 2.43 | 0.49 |
| 2:B:1513:U:O2' | 2:B:1514:G:H5' | 2.12 | 0.49 |
| 2:B:2567:G:H2' | 2:B:2568:U:C6 | 2.47 | 0.49 |
| 16:L:124:GLY:N | 16:L:143:GLU:CG | 2.74 | 0.49 |
| 20:J:36:LEU:HD21 | 20:J:122:LEU:HB2 | 1.95 | 0.49 |
| 2:B:2875:C:H4' | 7:P:1:SER:OG | 2.12 | 0.49 |
| 29:T:69:ARG:HB3 | 29:T:74:ILE:HD12 | 1.94 | 0.49 |
| 26:F:100:GLU:C | 26:F:102:LEU:H | 2.16 | 0.49 |
| 2:B:1443:U:H2' | 2:B:1444:G:C8 | 2.47 | 0.49 |
| 1:A:8:C:O2' | 22:O:40:ILE:HD13 | 2.12 | 0.49 |
| 22:O:49:VAL:HG21 | 22:O:82:ALA:HB2 | 1.95 | 0.49 |
| 2:B:873:C:H4' | 17:M:64:TRP:NE1 | 2.27 | 0.49 |
| 2:B:719:C:O2' | 2:B:720:U:H5' | 2.12 | 0.49 |
| 2:B:1505:A:H2' | 2:B:1506:U:C6 | 2.48 | 0.49 |
| 2:B:322:A:H2' | 8:E:163:ASN:HD21 | 1.77 | 0.49 |
| 2:B:2063:C:O2 | 2:B:2450:A:N1 | 2.46 | 0.49 |
| 24:S:13:SER:OG | 24:S:14:ALA:N | 2.46 | 0.49 |
| 2:B:1475:G:H1' | 2:B:1476:U:H5 | 1.77 | 0.49 |
| 2:B:2047:C:O2' | 2:B:2048:G:H5' | 2.11 | 0.49 |
| 2:B:1792:G:O2' | 2:B:1793:C:H5' | 2.13 | 0.49 |
| 2:B:2553:G:H2' | 2:B:2554:U:O4' | 2.13 | 0.49 |
| 2:B:1742:U:H2' | 2:B:1743:G:C8 | 2.48 | 0.49 |
| 16:L:81:ASP:CG | 16:L:100:ILE:HD11 | 2.33 | 0.49 |
| 14:V:31:TYR:HA | 14:V:93:ARG:CZ | 2.43 | 0.49 |
| 14:V:14:LYS:O | 14:V:18:ARG:HB2 | 2.12 | 0.49 |
| 2:B:545:U:H2' | 2:B:546:U:H4' | 1.95 | 0.49 |
| 21:N:101:GLY:O | 21:N:102:PHE:HB2 | 2.12 | 0.49 |
| 17:M:96:ILE:HD11 | 17:M:126:ILE:CD1 | 2.42 | 0.49 |
| 28:R:58:VAL:HG22 | 28:R:59:ILE:N | 2.26 | 0.49 |
| 22:O:35:ILE:O | 22:O:53:THR:HG23 | 2.13 | 0.49 |
| 7:P:89:GLY:N | 7:P:112:ARG:NH1 | 2.61 | 0.49 |
| 2:B:2230:G:H2' | 2:B:2231:U:C6 | 2.48 | 0.49 |
| 2:B:960:A:H61 | 17:M:82:MET:CE | 2.25 | 0.49 |
| 2:B:1043:C:H2' | 2:B:1044:C:O4' | 2.12 | 0.49 |
| 2:B:2315:G:H2' | 2:B:2316:G:H8 | 1.78 | 0.49 |
| 4:C:172:THR:HA | 4:C:182:LYS:HA | 1.95 | 0.49 |
| 5:D:107:VAL:H | 5:D:205:PRO:HA | 1.76 | 0.49 |
| 2:B:349:U:C2' | 2:B:350:G:H5' | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 29:T:23:ALA:C | 29:T:25:GLU:H | 2.15 | 0.49 |
| 3:I:17:ALA:O | 3:I:18:ASN:HB3 | 2.13 | 0.49 |
| 16:L:80:SER:HB3 | 16:L:115:GLU:CD | 2.33 | 0.49 |
| 2:B:182:A:H1' | 2:B:434:U:H5' | 1.94 | 0.49 |
| 10:O:41:HIS:HB2 | 21:N:99:LYS:O | 2.12 | 0.49 |
| 28:R:31:GLU:O | 28:R:62:GLU:HA | 2.13 | 0.49 |
| 14:V:5:ASN:HA | 14:V:64:VAL:O | 2.13 | 0.49 |
| 2:B:1516:G:O2' | 2:B:1517:G:H5' | 2.13 | 0.49 |
| 20:J:30:THR:HG23 | 20:J:31:GLU:H | 1.78 | 0.49 |
| 21:N:12:ARG:HG3 | 21:N:13:ASN:H | 1.77 | 0.49 |
| 2:B:1668:A:N3 | 2:B:1670:C:C4 | 2.81 | 0.49 |
| 4:C:12:ARG:HA | 4:C:15:VAL:HG23 | 1.94 | 0.49 |
| 2:B:1292:G:H2' | 2:B:1293:C:C6 | 2.48 | 0.49 |
| 2:B:57:C:H2' | 2:B:58:G:H8 | 1.77 | 0.49 |
| 4:C:86:ARG:NH1 | 4:C:86:ARG:HB3 | 2.28 | 0.49 |
| 22:O:112:GLU:O | 22:O:112:GLU:HG2 | 2.13 | 0.49 |
| 6:K:39:ILE:HD13 | 6:K:60:ALA:O | 2.13 | 0.49 |
| 2:B:146:A:H2' | 2:B:147:C:C6 | 2.48 | 0.49 |
| 2:B:820:A:H2' | 2:B:821:A:O4' | 2.13 | 0.49 |
| 2:B:1098:A:H2' | 3:I:3:LYS:C | 2.34 | 0.49 |
| 31:W:51:GLY:HA3 | 31:W:59:PHE:HB2 | 1.95 | 0.49 |
| 16:L:124:GLY:CA | 16:L:143:GLU:HG3 | 2.43 | 0.49 |
| 14:V:63:ILE:HD12 | 14:V:63:ILE:H | 1.77 | 0.49 |
| 14:V:42:LEU:HD11 | 14:V:89:ILE:HD11 | 1.95 | 0.49 |
| 5:D:20:VAL:HG13 | 6:K:72:PRO:HB3 | 1.95 | 0.49 |
| 2:B:2543:G:H2' | 2:B:2544:G:H8 | 1.78 | 0.49 |
| 28:R:72:VAL:CG2 | 28:R:89:HIS:HB3 | 2.39 | 0.49 |
| 2:B:1870:C:OP2 | 2:B:1870:C:H4' | 2.11 | 0.49 |
| 2:B:1803:A:H4' | 4:C:256:THR:OG1 | 2.13 | 0.49 |
| 14:V:65:VAL:C | 14:V:67:GLY:H | 2.16 | 0.49 |
| 18:X:23:ARG:O | 18:X:27:ASN:HB2 | 2.13 | 0.49 |
| 2:B:2449:U:H4' | 2:B:2450:A:OP1 | 2.13 | 0.49 |
| 4:C:211:ARG:C | 4:C:213:ARG:H | 2.16 | 0.49 |
| 1:A:12:C:N3 | 31:W:73:PRO:HG3 | 2.28 | 0.49 |
| 2:B:929:U:O2' | 2:B:930:G:H5' | 2.13 | 0.49 |
| 2:B:917:A:H2' | 2:B:918:A:O4' | 2.13 | 0.48 |
| 25:U:85:ARG:NH1 | 25:U:86:PHE:H | 2.10 | 0.48 |
| 7:P:54:LEU:HA | 7:P:76:HIS:CD2 | 2.47 | 0.48 |
| 7:P:74:GLN:O | 7:P:76:HIS:N | 2.46 | 0.48 |
| 14:V:57:TYR:HE2 | 17:M:136:MET:HE2 | 1.78 | 0.48 |
| 14:V:72:VAL:HG21 | 14:V:91:PHE:HB3 | 1.94 | 0.48 |
| 2:B:513:A:H8 | 2:B:513:A:O5' | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 17:M:19:GLY:CA | 17:M:97:GLN:HB2 | 2.38 | 0.48 |
| 21:N:79:LEU:HA | 21:N:83:LEU:CD1 | 2.43 | 0.48 |
| 26:F:137:PHE:N | 26:F:137:PHE:CD2 | 2.79 | 0.48 |
| 1:A:43:C:H1' | 26:F:91:ARG:HD2 | 1.95 | 0.48 |
| 24:S:25:ARG:HE | 24:S:74:ILE:CG2 | 2.25 | 0.48 |
| 6:K:54:LYS:H | 6:K:54:LYS:CD | 2.22 | 0.48 |
| 2:B:1080:A:H4' | 3:I:126:ARG:HD2 | 1.94 | 0.48 |
| 2:B:138:U:H5' | 29:T:1:MET:H1 | 1.76 | 0.48 |
| 25:U:80:ASP:HB2 | 25:U:96:LYS:H | 1.78 | 0.48 |
| 25:U:10:VAL:HA | 25:U:70:ALA:O | 2.13 | 0.48 |
| 2:B:2420:C:OP1 | 13:3:33:THR:HB | 2.13 | 0.48 |
| 2:B:2722:G:H2' | 2:B:2723:C:H6 | 1.76 | 0.48 |
| 14:V:61:LEU:O | 14:V:71:LYS:HA | 2.13 | 0.48 |
| 24:S:17:VAL:C | 24:S:19:LEU:N | 2.65 | 0.48 |
| 2:B:392:U:O2' | 2:B:393:C:H5' | 2.13 | 0.48 |
| 2:B:2813:A:H2' | 2:B:2814:A:H8 | 1.78 | 0.48 |
| 2:B:2784:U:H2' | 2:B:2785:C:C6 | 2.48 | 0.48 |
| 2:B:753:A:H2' | 2:B:754:U:H6 | 1.78 | 0.48 |
| 3:I:10:LEU:HD12 | 3:I:10:LEU:O | 2.12 | 0.48 |
| 2:B:538:A:H2' | 2:B:539:G:O4' | 2.12 | 0.48 |
| 26:F:74:ALA:C | 26:F:76:PHE:H | 2.16 | 0.48 |
| 27:G:120:ILE:HD11 | 27:G:132:LEU:CB | 2.43 | 0.48 |
| 26:F:96:TRP:HA | 26:F:99:PHE:HB3 | 1.94 | 0.48 |
| 2:B:1549:A:H2' | 2:B:1550:C:H6 | 1.77 | 0.48 |
| 19:H:111:ALA:O | 19:H:112:LYS:C | 2.50 | 0.48 |
| 27:G:148:ARG:HD3 | 27:G:152:ARG:NH2 | 2.28 | 0.48 |
| 25:U:11:ILE:O | 25:U:12:VAL:HB | 2.13 | 0.48 |
| 23:Q:26:ALA:HB1 | 23:Q:30:VAL:CB | 2.42 | 0.48 |
| 5:D:121:THR:HB | 5:D:127:PHE:CD1 | 2.48 | 0.48 |
| 13:3:3:ILE:HG23 | 16:L:48:ARG:HH12 | 1.78 | 0.48 |
| 28:R:36:ALA:HA | 28:R:58:VAL:HG23 | 1.95 | 0.48 |
| 2:B:246:C:O2' | 2:B:385:C:H4' | 2.14 | 0.48 |
| 2:B:2472:G:C2' | 2:B:2475:C:H42 | 2.26 | 0.48 |
| 2:B:1163:G:H4' | 28:R:92:TRP:HD1 | 1.76 | 0.48 |
| 2:B:1315:C:O2' | 2:B:1316:U:H5' | 2.13 | 0.48 |
| 8:E:196:VAL:O | 8:E:200:LEU:HD23 | 2.12 | 0.48 |
| 8:E:97:ASN:HD22 | 8:E:100:MET:HG3 | 1.78 | 0.48 |
| 2:B:1417:C:HO2' | 2:B:1587:G:HO2' | 1.60 | 0.48 |
| 2:B:688:U:O2' | 2:B:689:A:H5' | 2.12 | 0.48 |
| 6:K:25:LEU:HD12 | 6:K:38:ILE:HG22 | 1.94 | 0.48 |
| 2:B:2710:C:H2' | 2:B:2711:A:H8 | 1.77 | 0.48 |
| 2:B:575:A:O2' | 2:B:576:U:H5' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:550:C:H2' | 2:B:551:G:C8 | 2.48 | 0.48 |
| 16:L:81:ASP:HA | 16:L:84:LYS:CE | 2.43 | 0.48 |
| 16:L:81:ASP:HA | 16:L:84:LYS:HE3 | 1.95 | 0.48 |
| 23:Q:105:PHE:O | 23:Q:109:VAL:HG23 | 2.12 | 0.48 |
| 23:Q:91:ARG:NE | 28:R:11:GLN:HB2 | 2.28 | 0.48 |
| 28:R:39:LEU:HB2 | 28:R:49:ILE:HD11 | 1.96 | 0.48 |
| 14:V:63:ILE:O | 14:V:70:ILE:HG12 | 2.13 | 0.48 |
| 17:M:40:ARG:HH22 | 17:M:73:ILE:HD12 | 1.78 | 0.48 |
| 3:I:27:LEU:HD23 | 3:I:27:LEU:N | 2.21 | 0.48 |
| 30:Z:2:SER:O | 30:Z:3:ARG:C | 2.51 | 0.48 |
| 2:B:139:U:P | 2:B:139:U:H3' | 2.53 | 0.48 |
| 31:W:9:THR:OG1 | 31:W:10:ARG:N | 2.45 | 0.48 |
| 8:E:48:THR:C | 8:E:50:ALA:H | 2.16 | 0.48 |
| 8:E:113:VAL:HG22 | 8:E:118:LEU:HD12 | 1.95 | 0.48 |
| 2:B:2819:G:O2' | 2:B:2820:A:H5'' | 2.13 | 0.48 |
| 28:R:19:THR:HB | 28:R:96:VAL:O | 2.13 | 0.48 |
| 2:B:1387:A:H5' | 2:B:1469:A:H1' | 1.94 | 0.48 |
| 7:P:61:ARG:HD3 | 7:P:70:GLU:OE1 | 2.12 | 0.48 |
| 2:B:21:A:H2' | 2:B:22:C:C6 | 2.49 | 0.48 |
| 2:B:2756:U:H4' | 2:B:2757:A:OP1 | 2.13 | 0.48 |
| 2:B:847:U:H2' | 2:B:848:C:C6 | 2.47 | 0.48 |
| 14:V:80:HIS:HA | 14:V:87:GLN:OE1 | 2.13 | 0.48 |
| 2:B:2190:G:O2' | 2:B:2191:A:H5' | 2.13 | 0.48 |
| 2:B:1924:C:O2' | 2:B:1925:C:H5' | 2.13 | 0.48 |
| 1:A:87:U:H2' | 1:A:88:C:O5' | 2.13 | 0.48 |
| 2:B:106:C:H2' | 2:B:107:G:C8 | 2.48 | 0.48 |
| 2:B:2786:U:H5' | 5:D:70:LYS:HG3 | 1.95 | 0.48 |
| 2:B:2624:G:H1' | 10:0:18:HIS:HE1 | 1.78 | 0.48 |
| 2:B:167:A:H2' | 2:B:168:G:O4' | 2.14 | 0.48 |
| 2:B:2222:C:O2' | 2:B:2223:G:H5' | 2.14 | 0.48 |
| 4:C:141:HIS:CG | 4:C:142:ASN:N | 2.81 | 0.48 |
| 2:B:773:U:H4' | 4:C:45:ASN:O | 2.13 | 0.48 |
| 5:D:54:ALA:N | 5:D:76:GLY:HA2 | 2.29 | 0.48 |
| 6:K:71:ARG:HG2 | 6:K:105:ARG:HH21 | 1.79 | 0.48 |
| 26:F:32:LYS:H | 26:F:95:MET:HE1 | 1.78 | 0.48 |
| 2:B:2032:G:N2 | 5:D:151:THR:H | 2.11 | 0.48 |
| 2:B:2677:G:H2' | 2:B:2678:C:C6 | 2.48 | 0.48 |
| 2:B:2678:C:H2' | 2:B:2679:A:H8 | 1.77 | 0.48 |
| 26:F:64:PRO:HA | 26:F:88:VAL:HG21 | 1.93 | 0.48 |
| 15:2:33:ARG:HH21 | 15:2:33:ARG:CB | 2.24 | 0.48 |
| 2:B:1856:U:H2' | 2:B:1857:G:C5' | 2.42 | 0.48 |
| 2:B:1580:A:H2' | 2:B:1581:G:O4' | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:827:U:H5' | 2:B:828:U:O5' | 2.13 | 0.48 |
| 24:S:15:GLN:O | 24:S:19:LEU:HB2 | 2.14 | 0.48 |
| 2:B:2815:C:H2' | 2:B:2816:G:H8 | 1.79 | 0.48 |
| 2:B:263:G:H2' | 2:B:264:C:O4' | 2.13 | 0.48 |
| 2:B:1684:G:H2' | 2:B:1685:C:H6 | 1.78 | 0.48 |
| 11:4:13:ASN:HD22 | 11:4:13:ASN:N | 2.10 | 0.48 |
| 26:F:21:TYR:CE2 | 26:F:28:PRO:HD3 | 2.48 | 0.48 |
| 2:B:2847:U:H5'' | 7:P:94:ALA:CB | 2.43 | 0.48 |
| 5:D:133:THR:HG23 | 5:D:134:HIS:N | 2.29 | 0.48 |
| 18:X:12:GLU:HA | 18:X:15:ASN:ND2 | 2.19 | 0.48 |
| 2:B:1444:G:H2' | 2:B:1445:G:C8 | 2.48 | 0.48 |
| 29:T:2:ILE:HD13 | 29:T:2:ILE:H | 1.78 | 0.48 |
| 31:W:10:ARG:HD3 | 31:W:10:ARG:N | 2.29 | 0.48 |
| 2:B:182:A:O2' | 2:B:183:C:H5' | 2.13 | 0.48 |
| 6:K:119:ALA:O | 6:K:120:PRO:O | 2.32 | 0.48 |
| 2:B:288:U:H2' | 2:B:289:G:H8 | 1.78 | 0.48 |
| 2:B:973:A:OP1 | 2:B:973:A:H8 | 1.95 | 0.48 |
| 2:B:1727:C:H2' | 2:B:1728:C:C6 | 2.48 | 0.48 |
| 2:B:948:C:H2' | 2:B:949:G:H8 | 1.79 | 0.48 |
| 2:B:2462:C:H2' | 2:B:2463:C:C6 | 2.48 | 0.48 |
| 2:B:2751:G:H4' | 27:G:3:VAL:CG1 | 2.44 | 0.48 |
| 2:B:1259:G:H2' | 2:B:1260:A:H8 | 1.78 | 0.48 |
| 2:B:2617:U:O2' | 2:B:2618:G:H5' | 2.13 | 0.48 |
| 2:B:649:G:H2' | 2:B:650:C:C6 | 2.48 | 0.48 |
| 27:G:17:LYS:HG2 | 27:G:24:THR:HG23 | 1.96 | 0.48 |
| 28:R:4:VAL:CG2 | 28:R:39:LEU:HG | 2.44 | 0.48 |
| 2:B:773:U:H5'' | 2:B:773:U:H6 | 1.78 | 0.48 |
| 2:B:512:G:OP2 | 2:B:1235:G:H5' | 2.13 | 0.48 |
| 2:B:346:A:H2' | 2:B:347:A:C5' | 2.44 | 0.48 |
| 7:P:3:ILE:HD13 | 7:P:7:LEU:HD11 | 1.96 | 0.48 |
| 7:P:1:SER:H1 | 7:P:4:ILE:HD12 | 1.79 | 0.48 |
| 3:I:11:GLN:HA | 3:I:55:PRO:HA | 1.95 | 0.48 |
| 26:F:127:TYR:CB | 26:F:155:ILE:HD13 | 2.43 | 0.48 |
| 2:B:2444:G:OP2 | 8:E:63:LYS:HD2 | 2.12 | 0.48 |
| 2:B:1054:A:H2' | 2:B:1055:G:C8 | 2.48 | 0.48 |
| 7:P:91:VAL:HG11 | 7:P:96:LEU:CD1 | 2.41 | 0.48 |
| 12:1:9:LYS:HD3 | 12:1:9:LYS:N | 2.26 | 0.48 |
| 2:B:20:C:H2' | 2:B:21:A:H8 | 1.79 | 0.48 |
| 2:B:1124:G:O2' | 11:4:37:GLN:HG2 | 2.13 | 0.48 |
| 6:K:13:ASN:N | 6:K:100:PHE:HE1 | 2.12 | 0.48 |
| 2:B:1429:G:O2' | 2:B:1430:G:H5' | 2.12 | 0.48 |
| 2:B:222:A:N1 | 2:B:233:A:H5'' | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:150:U:H2' | 2:B:151:C:H6 | 1.76 | 0.48 |
| 2:B:2840:C:O2' | 2:B:2841:C:H5' | 2.13 | 0.48 |
| 2:B:2339:C:H2' | 2:B:2340:A:H8 | 1.77 | 0.48 |
| 2:B:1878:G:H2' | 2:B:1879:C:H6 | 1.78 | 0.48 |
| 2:B:2479:U:OP1 | 2:B:2537:U:H1' | 2.13 | 0.48 |
| 2:B:1458:U:H5'' | 2:B:1459:G:OP1 | 2.12 | 0.48 |
| 2:B:1459:G:H4' | 2:B:1461:C:H42 | 1.79 | 0.48 |
| 5:D:46:ARG:HH12 | 5:D:86:GLU:N | 2.12 | 0.48 |
| 2:B:2246:G:H2' | 2:B:2247:A:C8 | 2.48 | 0.48 |
| 2:B:2261:C:O2' | 2:B:2262:U:H5' | 2.14 | 0.48 |
| 9:Y:21:ALA:O | 9:Y:24:LEU:HB3 | 2.13 | 0.48 |
| 1:A:83:G:H4' | 9:Y:52:PHE:CD2 | 2.48 | 0.48 |
| 20:J:114:LEU:O | 20:J:118:MET:HG3 | 2.13 | 0.48 |
| 2:B:2000:C:O2' | 2:B:2001:C:H5' | 2.13 | 0.48 |
| 2:B:1099:G:N7 | 3:I:3:LYS:CD | 2.77 | 0.48 |
| 2:B:2271:G:H2' | 2:B:2272:U:O4' | 2.12 | 0.48 |
| 5:D:179:ARG:CB | 5:D:179:ARG:HH11 | 2.27 | 0.48 |
| 5:D:9:VAL:O | 5:D:9:VAL:HG13 | 2.12 | 0.48 |
| 26:F:113:PHE:CZ | 26:F:175:PRO:HB2 | 2.48 | 0.48 |
| 3:I:17:ALA:C | 3:I:19:PRO:HD3 | 2.34 | 0.48 |
| 4:C:75:ALA:HB2 | 4:C:95:TYR:HA | 1.94 | 0.48 |
| 8:E:134:LEU:O | 8:E:138:LEU:HG | 2.13 | 0.48 |
| 2:B:1843:C:H2' | 2:B:1844:C:C6 | 2.48 | 0.48 |
| 27:G:10:VAL:O | 27:G:10:VAL:HG12 | 2.14 | 0.48 |
| 17:M:33:LEU:HD22 | 17:M:128:THR:CB | 2.43 | 0.48 |
| 2:B:1315:C:H2' | 2:B:1316:U:H6 | 1.78 | 0.48 |
| 2:B:1153:C:H2' | 2:B:1154:G:O4' | 2.14 | 0.48 |
| 2:B:2458:G:H8 | 2:B:2459:A:H62 | 1.61 | 0.48 |
| 2:B:2199:A:H5' | 2:B:2200:C:OP2 | 2.13 | 0.48 |
| 2:B:1043:C:H2' | 2:B:1044:C:C6 | 2.48 | 0.48 |
| 2:B:1304:A:O2' | 2:B:1305:C:H5' | 2.14 | 0.48 |
| 2:B:2361:G:OP1 | 13:3:25:HIS:HA | 2.14 | 0.48 |
| 2:B:1636:U:H2' | 2:B:1637:A:H8 | 1.78 | 0.48 |
| 4:C:141:HIS:HB3 | 4:C:190:THR:OG1 | 2.13 | 0.48 |
| 6:K:34:GLY:O | 6:K:36:GLY:N | 2.46 | 0.48 |
| 19:H:4:ILE:HD13 | 19:H:44:ILE:HG22 | 1.94 | 0.48 |
| 14:V:77:VAL:HG11 | 17:M:136:MET:O | 2.13 | 0.48 |
| 27:G:116:LEU:N | 27:G:116:LEU:HD12 | 2.28 | 0.48 |
| 26:F:102:LEU:HD22 | 26:F:107:VAL:HG23 | 1.95 | 0.48 |
| 3:I:100:ILE:O | 3:I:139:VAL:HG13 | 2.14 | 0.48 |
| 17:M:26:VAL:CG2 | 17:M:133:LYS:HA | 2.43 | 0.48 |
| 2:B:2811:G:OP1 | 5:D:62:LYS:HD2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:E:148:ILE:HA | 8:E:187:VAL:HB | 1.96 | 0.48 |
| 2:B:1844:C:O3' | 4:C:255:LYS:HE2 | 2.13 | 0.48 |
| 30:Z:27:ARG:O | 30:Z:28:ARG:HB3 | 2.13 | 0.48 |
| 6:K:61:VAL:HG13 | 6:K:87:LEU:HD21 | 1.96 | 0.48 |
| 2:B:969:G:H2' | 2:B:970:U:H6 | 1.79 | 0.48 |
| 2:B:2394:C:H5'' | 16:L:63:LYS:HD3 | 1.95 | 0.48 |
| 2:B:2340:A:H2' | 2:B:2341:G:C8 | 2.49 | 0.48 |
| 2:B:1683:U:H2' | 2:B:1684:G:H8 | 1.77 | 0.48 |
| 2:B:1946:U:H2' | 2:B:1947:C:H6 | 1.78 | 0.48 |
| 18:X:22:LEU:CD1 | 18:X:23:ARG:HG2 | 2.44 | 0.48 |
| 2:B:493:G:H2' | 2:B:494:G:O4' | 2.14 | 0.48 |
| 2:B:1219:U:H2' | 2:B:1220:G:H8 | 1.78 | 0.48 |
| 2:B:69:C:O2' | 2:B:70:G:H5' | 2.13 | 0.48 |
| 12:1:18:HIS:NE2 | 12:1:40:PRO:HD2 | 2.28 | 0.48 |
| 2:B:1889:A:H2' | 2:B:1890:A:C8 | 2.49 | 0.48 |
| 2:B:1849:G:H2' | 2:B:1850:G:H8 | 1.79 | 0.48 |
| 4:C:221:GLY:C | 4:C:223:ALA:H | 2.16 | 0.48 |
| 6:K:103:VAL:HG23 | 6:K:122:VAL:O | 2.13 | 0.48 |
| 2:B:2398:U:H2' | 2:B:2399:G:H8 | 1.78 | 0.48 |
| 2:B:642:U:O2 | 2:B:644:A:H3' | 2.14 | 0.48 |
| 21:N:8:ARG:NH2 | 21:N:39:PRO:HB3 | 2.29 | 0.48 |
| 23:Q:51:GLN:O | 23:Q:55:GLN:HG3 | 2.14 | 0.48 |
| 14:V:24:ASN:O | 14:V:44:HIS:HB2 | 2.14 | 0.48 |
| 23:Q:4:LYS:NZ | 23:Q:7:VAL:HG13 | 2.28 | 0.48 |
| 4:C:166:ARG:CB | 4:C:171:VAL:HG22 | 2.43 | 0.48 |
| 29:T:25:GLU:HG3 | 29:T:29:THR:O | 2.14 | 0.48 |
| 2:B:1441:G:H2' | 2:B:1442:U:H6 | 1.79 | 0.48 |
| 2:B:357:C:H2' | 2:B:358:U:C5 | 2.49 | 0.48 |
| 19:H:110:VAL:O | 19:H:110:VAL:HG22 | 2.14 | 0.48 |
| 8:E:161:ALA:HB1 | 8:E:167:VAL:HG22 | 1.96 | 0.48 |
| 8:E:146:VAL:HG11 | 8:E:187:VAL:HG23 | 1.95 | 0.48 |
| 2:B:1873:G:O2' | 2:B:1874:C:H5' | 2.13 | 0.48 |
| 2:B:1874:C:H2' | 2:B:1875:G:O4' | 2.13 | 0.48 |
| 20:J:72:LYS:O | 20:J:73:VAL:HG13 | 2.13 | 0.48 |
| 1:A:30:C:H1' | 1:A:58:A:N1 | 2.28 | 0.48 |
| 12:1:43:ARG:NH2 | 12:1:43:ARG:HB3 | 2.28 | 0.48 |
| 22:O:30:ARG:HG2 | 22:O:102:ARG:HH11 | 1.77 | 0.48 |
| 24:S:81:SER:CB | 24:S:99:ARG:HA | 2.42 | 0.48 |
| 2:B:673:C:C2' | 2:B:674:G:H5' | 2.43 | 0.48 |
| 8:E:106:LYS:CE | 8:E:200:LEU:HB3 | 2.44 | 0.48 |
| 2:B:598:U:H2' | 2:B:599:A:H8 | 1.79 | 0.48 |
| 25:U:48:VAL:O | 25:U:48:VAL:HG13 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 27:G:72:ASN:O | 27:G:76:ILE:HG12 | 2.13 | 0.48 |
| 5:D:202:ILE:O | 5:D:202:ILE:HG22 | 2.13 | 0.48 |
| 2:B:188:G:OP1 | 30:Z:14:THR:HG22 | 2.12 | 0.48 |
| 2:B:965:C:O2' | 2:B:966:G:H5' | 2.13 | 0.48 |
| 31:W:36:ILE:HB | 31:W:39:GLN:NE2 | 2.28 | 0.48 |
| 27:G:24:THR:CG2 | 27:G:34:ARG:HB3 | 2.44 | 0.48 |
| 3:I:72:THR:CG2 | 3:I:112:LYS:HD2 | 2.44 | 0.48 |
| 24:S:66:ILE:HD13 | 24:S:66:ILE:N | 2.23 | 0.48 |
| 2:B:282:A:H2' | 2:B:283:G:O4' | 2.14 | 0.48 |
| 17:M:42:THR:OG1 | 17:M:45:GLN:HG3 | 2.14 | 0.48 |
| 5:D:90:PHE:HD2 | 5:D:94:GLN:HG3 | 1.78 | 0.48 |
| 2:B:163:C:O4' | 2:B:163:C:O2 | 2.32 | 0.48 |
| 12:1:34:GLU:HA | 12:1:48:TYR:O | 2.14 | 0.48 |
| 3:I:129:GLU:HB3 | 3:I:133:ARG:NH1 | 2.29 | 0.48 |
| 17:M:35:ALA:O | 17:M:36:VAL:HB | 2.13 | 0.48 |
| 26:F:134:GLN:OE1 | 26:F:136:ILE:HA | 2.13 | 0.48 |
| 22:O:88:LYS:HG2 | 22:O:89:ASP:N | 2.29 | 0.48 |
| 2:B:1229:C:H2' | 2:B:1230:A:C8 | 2.49 | 0.48 |
| 2:B:1729:U:H5'' | 2:B:1730:C:H4' | 1.95 | 0.48 |
| 2:B:1463:C:H2' | 2:B:1464:G:C8 | 2.49 | 0.48 |
| 2:B:1922:G:H2' | 2:B:1923:U:O4' | 2.13 | 0.48 |
| 2:B:1190:G:H5'' | 16:L:32:GLY:C | 2.34 | 0.48 |
| 18:X:1:MET:O | 18:X:5:GLU:HG2 | 2.13 | 0.48 |
| 2:B:2889:C:H2' | 2:B:2890:G:C8 | 2.48 | 0.48 |
| 2:B:2760:C:H2' | 2:B:2760:C:O2 | 2.13 | 0.48 |
| 13:3:35:LYS:HB2 | 13:3:40:LYS:HD3 | 1.95 | 0.48 |
| 24:S:42:LYS:O | 24:S:45:VAL:HG22 | 2.13 | 0.48 |
| 16:L:100:ILE:HG12 | 16:L:100:ILE:O | 2.14 | 0.47 |
| 16:L:92:LEU:CD2 | 16:L:124:GLY:HA3 | 2.44 | 0.47 |
| 28:R:6:GLN:HE21 | 28:R:6:GLN:C | 2.17 | 0.47 |
| 19:H:122:LEU:HD22 | 19:H:122:LEU:N | 2.29 | 0.47 |
| 19:H:89:LYS:HD2 | 19:H:89:LYS:H | 1.79 | 0.47 |
| 14:V:89:ILE:HD12 | 14:V:89:ILE:H | 1.79 | 0.47 |
| 2:B:2305:U:H2' | 2:B:2306:C:O4' | 2.14 | 0.47 |
| 27:G:84:LYS:HG3 | 27:G:131:VAL:CA | 2.43 | 0.47 |
| 8:E:40:ARG:NH2 | 8:E:92:HIS:NE2 | 2.62 | 0.47 |
| 2:B:544:C:H4' | 2:B:545:U:OP1 | 2.13 | 0.47 |
| 19:H:21:VAL:HG22 | 19:H:22:LYS:H | 1.79 | 0.47 |
| 3:I:23:VAL:HG12 | 3:I:27:LEU:HD21 | 1.95 | 0.47 |
| 25:U:15:GLY:O | 25:U:17:ASP:N | 2.46 | 0.47 |
| 12:1:22:THR:OG1 | 12:1:23:THR:N | 2.47 | 0.47 |
| 2:B:1798:U:H5'' | 4:C:257:ARG:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:1336:A:H3' | 2:B:1337:G:H8 | 1.78 | 0.47 |
| 2:B:2893:A:H4' | 2:B:2894:G:O5' | 2.13 | 0.47 |
| 14:V:66:ASP:OD1 | 14:V:68:LYS:HD3 | 2.14 | 0.47 |
| 2:B:38:A:N3 | 8:E:43:THR:HB | 2.29 | 0.47 |
| 2:B:1463:C:H2' | 2:B:1464:G:H8 | 1.78 | 0.47 |
| 2:B:2438:U:O3' | 2:B:2439:A:H3' | 2.14 | 0.47 |
| 2:B:2291:U:O2' | 2:B:2374:C:H1' | 2.14 | 0.47 |
| 2:B:1656:C:H2' | 2:B:1657:U:C6 | 2.49 | 0.47 |
| 2:B:1513:U:H2' | 2:B:1514:G:C8 | 2.49 | 0.47 |
| 2:B:576:U:H2' | 2:B:577:G:C8 | 2.48 | 0.47 |
| 2:B:1979:U:O2' | 2:B:1980:G:H5' | 2.13 | 0.47 |
| 2:B:798:G:OP2 | 8:E:56:GLY:HA3 | 2.14 | 0.47 |
| 23:Q:18:LYS:C | 23:Q:20:ALA:H | 2.18 | 0.47 |
| 2:B:1560:G:H2' | 2:B:1561:C:H6 | 1.77 | 0.47 |
| 4:C:106:PRO:O | 4:C:109:LEU:HB3 | 2.14 | 0.47 |
| 26:F:92:GLY:HA2 | 26:F:95:MET:HE3 | 1.95 | 0.47 |
| 2:B:566:U:OP1 | 16:L:29:LYS:HD3 | 2.13 | 0.47 |
| 19:H:14:SER:HB3 | 19:H:17:ASP:OD1 | 2.14 | 0.47 |
| 30:Z:64:ILE:O | 30:Z:68:LEU:HG | 2.14 | 0.47 |
| 25:U:3:LYS:CB | 25:U:82:VAL:HG21 | 2.44 | 0.47 |
| 17:M:26:VAL:HA | 17:M:66:ARG:HH21 | 1.79 | 0.47 |
| 2:B:1654:A:H2' | 2:B:1655:A:H8 | 1.79 | 0.47 |
| 21:N:97:ILE:HD13 | 21:N:99:LYS:HG3 | 1.95 | 0.47 |
| 5:D:33:ARG:HE | 5:D:74:GLU:HB3 | 1.79 | 0.47 |
| 2:B:666:A:O2' | 2:B:667:U:H5' | 2.13 | 0.47 |
| 26:F:45:ASP:O | 26:F:46:LYS:HB2 | 2.14 | 0.47 |
| 27:G:10:VAL:CG2 | 27:G:48:THR:HA | 2.44 | 0.47 |
| 6:K:11:ALA:HB3 | 6:K:85:VAL:HG23 | 1.95 | 0.47 |
| 2:B:7:G:H4' | 20:J:15:TRP:CZ2 | 2.48 | 0.47 |
| 1:A:94:A:O2' | 1:A:95:U:H5' | 2.14 | 0.47 |
| 5:D:102:ALA:HA | 5:D:180:VAL:HG21 | 1.95 | 0.47 |
| 2:B:1259:G:H2' | 2:B:1260:A:C8 | 2.49 | 0.47 |
| 1:A:112:G:O2' | 1:A:113:C:H5' | 2.13 | 0.47 |
| 2:B:2516:A:O2' | 2:B:2517:C:H5' | 2.14 | 0.47 |
| 29:T:60:THR:HA | 29:T:82:LYS:O | 2.15 | 0.47 |
| 2:B:1032:A:H1' | 11:4:23:ILE:HD13 | 1.96 | 0.47 |
| 2:B:218:A:O2' | 2:B:219:A:H5' | 2.14 | 0.47 |
| 2:B:2643:G:H2' | 2:B:2644:G:O4' | 2.13 | 0.47 |
| 3:I:2:LYS:O | 3:I:3:LYS:HG3 | 2.13 | 0.47 |
| 2:B:1175:A:H3' | 2:B:1176:U:C5' | 2.33 | 0.47 |
| 2:B:2875:C:H2' | 2:B:2876:G:C8 | 2.48 | 0.47 |
| 5:D:9:VAL:HG22 | 5:D:9:VAL:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 19:H:46:PHE:O | 19:H:50:ARG:HB2 | 2.14 | 0.47 |
| 5:D:114:LYS:HE3 | 5:D:116:LYS:HG2 | 1.95 | 0.47 |
| 5:D:121:THR:C | 5:D:123:LYS:H | 2.18 | 0.47 |
| 26:F:55:ASP:OD2 | 26:F:149:ARG:HG3 | 2.14 | 0.47 |
| 26:F:41:GLU:O | 26:F:43:ILE:N | 2.45 | 0.47 |
| 1:A:106:G:H2' | 1:A:107:G:C8 | 2.50 | 0.47 |
| 28:R:70:GLU:O | 28:R:90:ARG:HA | 2.13 | 0.47 |
| 2:B:2213:U:O2 | 2:B:2213:U:C2' | 2.62 | 0.47 |
| 2:B:2296:U:H4' | 2:B:2297:A:OP1 | 2.13 | 0.47 |
| 2:B:2773:C:O2' | 2:B:2774:C:H5' | 2.13 | 0.47 |
| 17:M:105:MET:HB2 | 17:M:117:PHE:CZ | 2.49 | 0.47 |
| 2:B:265:A:O2' | 2:B:266:G:C4' | 2.61 | 0.47 |
| 2:B:2600:A:O2' | 2:B:2601:C:H5' | 2.14 | 0.47 |
| 2:B:2309:A:H2' | 2:B:2310:C:C6 | 2.49 | 0.47 |
| 6:K:109:SER:OG | 6:K:111:LYS:HG2 | 2.14 | 0.47 |
| 1:A:55:U:H2' | 1:A:56:G:H8 | 1.78 | 0.47 |
| 2:B:2247:A:H2' | 2:B:2248:C:H6 | 1.79 | 0.47 |
| 2:B:2046:G:H5' | 10:O:15:ARG:HG3 | 1.95 | 0.47 |
| 6:K:53:LYS:HD3 | 6:K:53:LYS:H | 1.79 | 0.47 |
| 2:B:426:C:O2' | 2:B:427:U:H5' | 2.13 | 0.47 |
| 2:B:620:G:N3 | 2:B:620:G:H5' | 2.29 | 0.47 |
| 2:B:1936:A:H2 | 2:B:1943:U:O4 | 1.98 | 0.47 |
| 2:B:189:G:H2' | 2:B:205:G:H22 | 1.80 | 0.47 |
| 2:B:189:G:H2' | 2:B:205:G:N2 | 2.30 | 0.47 |
| 23:Q:40:LYS:HA | 23:Q:43:GLN:OE1 | 2.14 | 0.47 |
| 20:J:134:ALA:HB3 | 20:J:135:GLN:NE2 | 2.29 | 0.47 |
| 2:B:2852:G:H2' | 2:B:2853:C:O4' | 2.13 | 0.47 |
| 17:M:61:GLY:HA2 | 17:M:107:GLY:HA3 | 1.97 | 0.47 |
| 2:B:2778:A:O2' | 2:B:2781:A:H5' | 2.14 | 0.47 |
| 2:B:919:U:H2' | 2:B:920:A:H8 | 1.77 | 0.47 |
| 4:C:185:ALA:C | 4:C:187:CYS:H | 2.17 | 0.47 |
| 17:M:38:ARG:CA | 17:M:98:PRO:HD3 | 2.44 | 0.47 |
| 29:T:21:SER:HB3 | 29:T:31:VAL:HG22 | 1.96 | 0.47 |
| 27:G:84:LYS:HG3 | 27:G:131:VAL:CB | 2.44 | 0.47 |
| 17:M:71:LYS:HE3 | 17:M:73:ILE:CD1 | 2.37 | 0.47 |
| 26:F:2:LYS:CD | 26:F:100:GLU:HG2 | 2.44 | 0.47 |
| 2:B:2531:A:P | 27:G:174:LYS:HB3 | 2.54 | 0.47 |
| 2:B:2443:C:H2' | 2:B:2444:G:H8 | 1.78 | 0.47 |
| 2:B:1103:A:H3' | 2:B:1104:C:H6 | 1.79 | 0.47 |
| 3:I:18:ASN:N | 3:I:19:PRO:CD | 2.77 | 0.47 |
| 9:Y:6:ILE:N | 9:Y:6:ILE:HD13 | 2.29 | 0.47 |
| 27:G:86:LEU:HG | 27:G:163:TYR:HD1 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 7:P:47:ILE:HG13 | 7:P:48:ALA:N | 2.28 | 0.47 |
| 25:U:66:VAL:O | 25:U:69:VAL:HG22 | 2.15 | 0.47 |
| 2:B:2591:C:OP1 | 4:C:237:ARG:HG3 | 2.13 | 0.47 |
| 8:E:47:LYS:HA | 8:E:51:GLU:HG3 | 1.96 | 0.47 |
| 2:B:2415:G:H2' | 2:B:2416:C:H6 | 1.80 | 0.47 |
| 2:B:2468:A:H2' | 2:B:2476:A:C6 | 2.49 | 0.47 |
| 2:B:655:A:H4' | 2:B:656:G:H5' | 1.96 | 0.47 |
| 2:B:1409:U:H2' | 2:B:1410:G:H8 | 1.78 | 0.47 |
| 2:B:877:A:C2' | 2:B:900:A:H61 | 2.28 | 0.47 |
| 2:B:2734:A:C2' | 2:B:2735:G:H5' | 2.45 | 0.47 |
| 27:G:37:ASN:HD21 | 27:G:40:VAL:N | 2.12 | 0.47 |
| 2:B:2187:U:H2' | 2:B:2188:U:C5 | 2.49 | 0.47 |
| 2:B:1130:U:C2 | 2:B:2025:C:H5'' | 2.49 | 0.47 |
| 2:B:1315:C:H2' | 2:B:1316:U:C6 | 2.50 | 0.47 |
| 29:T:62:VAL:HG12 | 29:T:63:VAL:N | 2.30 | 0.47 |
| 7:P:31:VAL:HG12 | 7:P:38:ARG:O | 2.13 | 0.47 |
| 2:B:1824:G:O2' | 4:C:251:THR:HG21 | 2.15 | 0.47 |
| 2:B:1403:A:H2' | 2:B:1404:C:H6 | 1.78 | 0.47 |
| 23:Q:70:GLN:HA | 23:Q:70:GLN:NE2 | 2.29 | 0.47 |
| 24:S:88:ARG:N | 24:S:92:ARG:O | 2.47 | 0.47 |
| 2:B:2730:C:H2' | 2:B:2731:G:H8 | 1.80 | 0.47 |
| 14:V:10:LYS:HG2 | 14:V:11:GLU:HG3 | 1.96 | 0.47 |
| 2:B:2267:A:C8 | 2:B:2267:A:O5' | 2.67 | 0.47 |
| 16:L:93:ASN:HB2 | 16:L:94:THR:H | 1.49 | 0.47 |
| 8:E:158:PHE:HA | 8:E:169:VAL:HG21 | 1.96 | 0.47 |
| 23:Q:91:ARG:NE | 23:Q:94:LEU:HD23 | 2.26 | 0.47 |
| 22:O:20:GLU:OE2 | 22:O:21:LEU:HG | 2.15 | 0.47 |
| 5:D:77:ARG:HB2 | 5:D:80:TRP:HH2 | 1.79 | 0.47 |
| 2:B:283:G:H2' | 2:B:284:U:O4' | 2.14 | 0.47 |
| 2:B:2313:C:H2' | 2:B:2314:A:H8 | 1.78 | 0.47 |
| 26:F:100:GLU:C | 26:F:102:LEU:N | 2.65 | 0.47 |
| 9:Y:29:ARG:H | 9:Y:33:HIS:CD2 | 2.32 | 0.47 |
| 7:P:20:ARG:HH21 | 7:P:20:ARG:HG2 | 1.79 | 0.47 |
| 17:M:126:ILE:N | 17:M:126:ILE:HD12 | 2.22 | 0.47 |
| 2:B:2809:A:N6 | 2:B:2891:U:H4' | 2.29 | 0.47 |
| 22:O:88:LYS:HG2 | 22:O:116:GLN:HB2 | 1.95 | 0.47 |
| 31:W:44:PHE:HB3 | 31:W:78:PHE:CD1 | 2.50 | 0.47 |
| 8:E:136:GLN:NE2 | 8:E:139:LYS:HD3 | 2.29 | 0.47 |
| 2:B:2872:A:H1' | 2:B:2873:A:C8 | 2.50 | 0.47 |
| 2:B:1351:C:H2' | 2:B:1352:U:O4' | 2.14 | 0.47 |
| 2:B:825:A:H2' | 2:B:826:U:O4' | 2.15 | 0.47 |
| 11:4:16:ILE:HG12 | 11:4:25:VAL:HG22 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:I:37:PHE:HB2 | 3:I:66:PHE:CE2 | 2.49 | 0.47 |
| 2:B:2054:A:H2' | 10:0:4:GLN:OE1 | 2.14 | 0.47 |
| 2:B:549:G:H2' | 20:J:2:LYS:HE3 | 1.96 | 0.47 |
| 2:B:1309:G:OP1 | 15:2:9:VAL:HG12 | 2.15 | 0.47 |
| 4:C:33:LEU:CD2 | 4:C:62:ARG:HG3 | 2.44 | 0.47 |
| 2:B:2888:C:H2' | 2:B:2889:C:C6 | 2.49 | 0.47 |
| 4:C:177:SER:O | 4:C:270:ARG:HG3 | 2.15 | 0.47 |
| 2:B:1930:G:N2 | 2:B:1968:G:H2' | 2.30 | 0.47 |
| 6:K:31:ARG:HB3 | 6:K:32:TYR:CE1 | 2.49 | 0.47 |
| 28:R:5:PHE:O | 28:R:11:GLN:HA | 2.15 | 0.47 |
| 7:P:3:ILE:HD13 | 7:P:3:ILE:C | 2.35 | 0.47 |
| 2:B:2466:C:OP1 | 11:4:4:ARG:HD2 | 2.13 | 0.47 |
| 27:G:120:ILE:HD13 | 27:G:121:THR:N | 2.29 | 0.47 |
| 26:F:29:ARG:CB | 26:F:29:ARG:HH11 | 2.26 | 0.47 |
| 16:L:79:LEU:H | 16:L:113:ALA:CB | 2.27 | 0.47 |
| 19:H:112:LYS:HG3 | 19:H:112:LYS:O | 2.15 | 0.47 |
| 27:G:148:ARG:HD3 | 27:G:152:ARG:HD3 | 1.95 | 0.47 |
| 27:G:153:PRO:HB3 | 27:G:158:GLY:HA2 | 1.97 | 0.47 |
| 2:B:1187:G:HO2' | 2:B:1188:U:H6 | 1.58 | 0.47 |
| 2:B:1599:U:H2' | 2:B:1600:C:H6 | 1.75 | 0.47 |
| 2:B:2394:C:H6 | 2:B:2394:C:O5' | 1.98 | 0.47 |
| 2:B:1131:G:N2 | 2:B:2024:G:H21 | 2.11 | 0.47 |
| 4:C:51:ARG:HH21 | 4:C:246:PRO:HG2 | 1.78 | 0.47 |
| 16:L:47:ARG:CG | 16:L:50:PHE:HB2 | 2.44 | 0.47 |
| 4:C:52:HIS:O | 4:C:53:ILE:HB | 2.13 | 0.47 |
| 27:G:61:TRP:HA | 27:G:61:TRP:CE3 | 2.48 | 0.47 |
| 4:C:86:ARG:CZ | 4:C:86:ARG:HB3 | 2.45 | 0.47 |
| 2:B:1559:U:H4' | 2:B:1560:G:OP2 | 2.14 | 0.47 |
| 22:O:45:SER:HB2 | 22:O:46:GLU:OE1 | 2.14 | 0.47 |
| 2:B:1539:U:H3' | 2:B:1540:G:H8 | 1.78 | 0.47 |
| 2:B:2331:G:C4' | 31:W:39:GLN:HA | 2.45 | 0.47 |
| 31:W:24:ARG:HB2 | 31:W:65:LYS:HB3 | 1.96 | 0.47 |
| 2:B:2352:A:C2 | 31:W:29:SER:HB3 | 2.50 | 0.47 |
| 27:G:34:ARG:HD3 | 27:G:34:ARG:H | 1.80 | 0.47 |
| 19:H:119:ASN:O | 19:H:121:VAL:HG22 | 2.14 | 0.47 |
| 19:H:121:VAL:HG12 | 19:H:123:ARG:CZ | 2.45 | 0.47 |
| 7:P:50:ARG:CD | 7:P:56:SER:HB3 | 2.45 | 0.47 |
| 3:I:52:LEU:HD13 | 3:I:81:LYS:HZ3 | 1.79 | 0.47 |
| 3:I:75:ALA:O | 3:I:79:LEU:HG | 2.14 | 0.47 |
| 5:D:91:THR:HG23 | 5:D:92:VAL:N | 2.22 | 0.47 |
| 29:T:18:GLU:O | 29:T:20:ALA:N | 2.47 | 0.47 |
| 29:T:1:MET:HE3 | 29:T:4:GLU:OE2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 28:R:62:GLU:O | 28:R:96:VAL:HA | 2.15 | 0.47 |
| 26:F:147:ARG:NH1 | 26:F:147:ARG:HB3 | 2.29 | 0.47 |
| 18:X:13:GLU:HB3 | 18:X:57:LEU:HD21 | 1.96 | 0.47 |
| 18:X:9:LYS:O | 18:X:13:GLU:HG2 | 2.15 | 0.47 |
| 14:V:3:THR:HA | 14:V:62:THR:HG1 | 1.79 | 0.47 |
| 1:A:30:C:O2 | 1:A:30:C:H2' | 2.14 | 0.47 |
| 2:B:974:G:H1' | 2:B:975:A:C8 | 2.49 | 0.47 |
| 2:B:459:U:O2' | 2:B:460:A:H5' | 2.15 | 0.47 |
| 22:O:30:ARG:CG | 22:O:102:ARG:HH11 | 2.28 | 0.47 |
| 11:4:25:VAL:O | 11:4:26:ILE:HD13 | 2.14 | 0.47 |
| 2:B:968:C:H2' | 2:B:969:G:C8 | 2.49 | 0.47 |
| 2:B:839:U:H2' | 2:B:840:C:C6 | 2.48 | 0.47 |
| 8:E:130:LYS:HB2 | 8:E:133:LEU:HG | 1.95 | 0.47 |
| 2:B:2349:G:OP2 | 13:3:41:ARG:HD3 | 2.14 | 0.47 |
| 18:X:22:LEU:O | 18:X:24:GLU:N | 2.47 | 0.47 |
| 28:R:79:ARG:O | 28:R:81:LYS:HG2 | 2.15 | 0.47 |
| 2:B:2888:C:H2' | 2:B:2889:C:H6 | 1.80 | 0.47 |
| 1:A:54:G:H21 | 26:F:25:MET:HE3 | 1.79 | 0.47 |
| 2:B:2094:A:H2' | 2:B:2095:A:H8 | 1.79 | 0.47 |
| 2:B:2096:C:H2' | 2:B:2097:A:H8 | 1.80 | 0.47 |
| 2:B:2223:G:H2' | 2:B:2224:G:H5' | 1.97 | 0.47 |
| 2:B:518:G:H2' | 2:B:519:U:C6 | 2.50 | 0.47 |
| 2:B:196:A:H2' | 2:B:196:A:N3 | 2.30 | 0.47 |
| 7:P:103:THR:HG22 | 7:P:104:GLY:H | 1.80 | 0.47 |
| 21:N:41:ALA:C | 21:N:43:GLU:N | 2.67 | 0.47 |
| 10:0:54:ILE:H | 21:N:118:ARG:HH12 | 1.63 | 0.47 |
| 16:L:110:VAL:HB | 16:L:127:VAL:HG23 | 1.96 | 0.47 |
| 14:V:48:MET:SD | 14:V:85:LYS:HA | 2.54 | 0.47 |
| 21:N:63:ARG:O | 21:N:66:ALA:HB3 | 2.14 | 0.47 |
| 2:B:744:U:H2' | 2:B:745:G:O4' | 2.15 | 0.47 |
| 2:B:125:A:O2' | 15:2:13:ASN:HB3 | 2.14 | 0.47 |
| 30:Z:35:SER:CA | 30:Z:50:ARG:HA | 2.41 | 0.47 |
| 2:B:2769:U:O2' | 2:B:2770:G:H5' | 2.14 | 0.47 |
| 19:H:125:THR:HA | 19:H:146:VAL:CB | 2.40 | 0.47 |
| 25:U:9:GLU:HG3 | 25:U:21:ARG:HD2 | 1.96 | 0.47 |
| 17:M:96:ILE:HD11 | 17:M:126:ILE:HD13 | 1.96 | 0.47 |
| 23:Q:27:ARG:HG3 | 23:Q:27:ARG:HH11 | 1.79 | 0.47 |
| 2:B:2040:G:H2' | 2:B:2041:U:O4' | 2.14 | 0.47 |
| 26:F:45:ASP:C | 26:F:47:LYS:H | 2.18 | 0.47 |
| 2:B:1372:U:H1' | 2:B:2214:C:C4 | 2.49 | 0.47 |
| 24:S:17:VAL:HG13 | 24:S:43:ALA:HB1 | 1.97 | 0.47 |
| 18:X:41:HIS:O | 18:X:44:LYS:HB3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:299:A:N6 | 2:B:322:A:O2' | 2.47 | 0.47 |
| 2:B:522:A:H2' | 2:B:523:C:H6 | 1.79 | 0.47 |
| 24:S:95:ARG:O | 24:S:96:ILE:HG22 | 2.15 | 0.47 |
| 2:B:510:C:O2' | 2:B:1236:G:H5' | 2.15 | 0.47 |
| 7:P:103:THR:HG22 | 7:P:104:GLY:N | 2.30 | 0.47 |
| 20:J:34:ARG:HG2 | 20:J:39:LYS:HB3 | 1.97 | 0.47 |
| 2:B:671:C:O2' | 2:B:672:C:H5' | 2.15 | 0.47 |
| 2:B:381:G:OP1 | 30:Z:18:ARG:HD2 | 2.14 | 0.47 |
| 2:B:1831:G:H2' | 2:B:1832:C:C6 | 2.50 | 0.47 |
| 25:U:85:ARG:HH11 | 25:U:86:PHE:N | 2.12 | 0.47 |
| 2:B:350:G:H2' | 2:B:351:C:H6 | 1.80 | 0.47 |
| 6:K:19:VAL:CB | 6:K:41:ILE:HD11 | 2.45 | 0.47 |
| 22:O:18:LEU:HD23 | 22:O:25:ARG:HD2 | 1.95 | 0.47 |
| 1:A:33:G:O2' | 1:A:34:A:H5' | 2.15 | 0.47 |
| 16:L:111:ILE:HG22 | 16:L:112:LEU:N | 2.29 | 0.47 |
| 19:H:69:ALA:HA | 19:H:140:ALA:HB2 | 1.96 | 0.47 |
| 2:B:2472:G:O6 | 2:B:2476:A:H4' | 2.15 | 0.47 |
| 28:R:83:TYR:HE2 | 28:R:85:LYS:HE3 | 1.80 | 0.47 |
| 2:B:992:C:O2' | 2:B:993:G:H5' | 2.15 | 0.47 |
| 2:B:416:U:O2' | 2:B:417:C:H5' | 2.15 | 0.47 |
| 2:B:2007:U:O2' | 2:B:2008:C:H5' | 2.15 | 0.47 |
| 2:B:1947:C:H2' | 2:B:1948:G:H8 | 1.80 | 0.47 |
| 1:A:55:U:H2' | 1:A:56:G:C8 | 2.50 | 0.47 |
| 4:C:202:ARG:HH21 | 4:C:202:ARG:HB2 | 1.79 | 0.47 |
| 2:B:757:G:H2' | 2:B:758:C:H5' | 1.96 | 0.47 |
| 16:L:142:ILE:HD12 | 16:L:142:ILE:N | 2.30 | 0.47 |
| 1:A:76:G:H5'' | 14:V:17:SER:OG | 2.15 | 0.47 |
| 2:B:225:C:O2' | 2:B:226:A:H5' | 2.15 | 0.47 |
| 24:S:5:ALA:HB3 | 24:S:54:ALA:HB2 | 1.96 | 0.47 |
| 2:B:466:A:N3 | 2:B:683:U:H1' | 2.30 | 0.47 |
| 31:W:49:ASN:O | 31:W:50:VAL:HG13 | 2.15 | 0.47 |
| 23:Q:93:ILE:HG23 | 23:Q:94:LEU:HD22 | 1.97 | 0.47 |
| 4:C:102:TYR:C | 4:C:103:ILE:HG13 | 2.36 | 0.47 |
| 2:B:2886:A:N6 | 10:0:39:ARG:CZ | 2.78 | 0.47 |
| 2:B:2845:U:O2' | 2:B:2846:G:H5' | 2.14 | 0.47 |
| 30:Z:71:LEU:CD1 | 30:Z:76:GLU:HG2 | 2.45 | 0.47 |
| 1:A:6:G:H2' | 1:A:7:G:C8 | 2.50 | 0.47 |
| 2:B:2645:G:H4' | 2:B:2732:G:H2' | 1.97 | 0.47 |
| 6:K:70:ARG:CB | 6:K:76:VAL:HG22 | 2.41 | 0.47 |
| 2:B:2417:C:O2' | 2:B:2418:A:H5' | 2.14 | 0.47 |
| 2:B:532:A:H4' | 2:B:533:G:C8 | 2.49 | 0.47 |
| 28:R:15:SER:H | 28:R:18:GLN:CD | 2.18 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:975:A:H1' | 2:B:990:A:C2 | 2.50 | 0.47 |
| 2:B:717:C:C3' | 2:B:718:A:H5'' | 2.44 | 0.47 |
| 8:E:30:GLN:HG2 | 8:E:30:GLN:O | 2.15 | 0.47 |
| 5:D:170:VAL:O | 5:D:170:VAL:HG23 | 2.14 | 0.47 |
| 1:A:24:G:O2' | 1:A:27:C:N4 | 2.48 | 0.47 |
| 2:B:322:A:H5' | 2:B:340:A:C1' | 2.45 | 0.47 |
| 4:C:33:LEU:O | 4:C:34:GLU:HB3 | 2.14 | 0.47 |
| 2:B:2098:U:H2' | 2:B:2099:U:H1' | 1.97 | 0.47 |
| 2:B:1860:G:H2' | 2:B:1861:G:H8 | 1.80 | 0.47 |
| 2:B:2223:G:C2' | 2:B:2224:G:H5' | 2.44 | 0.47 |
| 2:B:2539:C:O2' | 2:B:2540:C:H5' | 2.15 | 0.47 |
| 2:B:259:G:O2' | 2:B:260:G:H5' | 2.15 | 0.47 |
| 24:S:70:LYS:HD3 | 24:S:110:ARG:OXT | 2.15 | 0.47 |
| 2:B:1477:A:H2' | 2:B:1478:G:O4' | 2.15 | 0.47 |
| 2:B:2332:C:H1' | 2:B:2336:A:N7 | 2.30 | 0.46 |
| 23:Q:85:ALA:O | 23:Q:86:SER:C | 2.54 | 0.46 |
| 23:Q:96:ASP:C | 23:Q:98:ALA:N | 2.69 | 0.46 |
| 19:H:4:ILE:HD12 | 19:H:4:ILE:N | 2.31 | 0.46 |
| 14:V:44:HIS:HE1 | 14:V:86:LEU:N | 2.09 | 0.46 |
| 14:V:51:GLN:NE2 | 14:V:79:ARG:HH22 | 2.12 | 0.46 |
| 29:T:44:LYS:HG3 | 29:T:55:VAL:HG11 | 1.95 | 0.46 |
| 2:B:1454:C:H5' | 21:N:63:ARG:CZ | 2.46 | 0.46 |
| 26:F:110:ILE:CG2 | 26:F:113:PHE:HB3 | 2.44 | 0.46 |
| 23:Q:79:ILE:O | 23:Q:79:ILE:HD13 | 2.14 | 0.46 |
| 2:B:2070:A:H2' | 2:B:2071:A:C8 | 2.50 | 0.46 |
| 30:Z:59:ILE:CG2 | 30:Z:64:ILE:HG13 | 2.44 | 0.46 |
| 2:B:138:U:H6 | 2:B:138:U:O5' | 1.98 | 0.46 |
| 2:B:182:A:H2' | 2:B:183:C:H6 | 1.79 | 0.46 |
| 10:0:41:HIS:O | 10:0:42:ILE:O | 2.33 | 0.46 |
| 11:4:11:CYS:SG | 11:4:12:ARG:N | 2.89 | 0.46 |
| 13:3:54:LEU:HG | 13:3:58:ILE:HD11 | 1.97 | 0.46 |
| 1:A:28:C:H5' | 1:A:29:A:OP2 | 2.14 | 0.46 |
| 22:O:67:ASN:O | 22:O:69:ASP:N | 2.48 | 0.46 |
| 22:O:30:ARG:NH2 | 22:O:103:VAL:HG23 | 2.31 | 0.46 |
| 2:B:1730:C:O2' | 2:B:1731:G:N2 | 2.48 | 0.46 |
| 13:3:41:ARG:HG3 | 13:3:44:ARG:NH2 | 2.29 | 0.46 |
| 19:H:128:HIS:C | 19:H:143:ILE:HG23 | 2.36 | 0.46 |
| 10:0:50:GLY:C | 10:0:51:ARG:HG2 | 2.35 | 0.46 |
| 2:B:2710:C:H2' | 2:B:2711:A:C8 | 2.50 | 0.46 |
| 3:I:69:VAL:O | 3:I:69:VAL:HG23 | 2.14 | 0.46 |
| 19:H:15:LEU:HD13 | 19:H:15:LEU:C | 2.35 | 0.46 |
| 21:N:82:GLU:C | 21:N:84:GLY:H | 2.18 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2822:G:H5'' | 5:D:164:GLN:OE1 | 2.15 | 0.46 |
| 1:A:109:A:H2' | 1:A:110:C:C6 | 2.50 | 0.46 |
| 27:G:42:VAL:HA | 27:G:51:PHE:HA | 1.98 | 0.46 |
| 20:J:29:ALA:O | 20:J:32:LEU:HB2 | 2.15 | 0.46 |
| 2:B:2683:C:H5'' | 7:P:55:HIS:HB3 | 1.97 | 0.46 |
| 2:B:77:G:O2' | 2:B:78:U:H5' | 2.15 | 0.46 |
| 29:T:22:THR:O | 29:T:26:LYS:HG2 | 2.16 | 0.46 |
| 4:C:89:ASN:O | 4:C:105:ALA:HB3 | 2.14 | 0.46 |
| 2:B:443:A:H1' | 2:B:1201:U:O4' | 2.16 | 0.46 |
| 6:K:19:VAL:C | 6:K:41:ILE:HD11 | 2.35 | 0.46 |
| 31:W:44:PHE:O | 31:W:78:PHE:HA | 2.15 | 0.46 |
| 2:B:1348:C:H2' | 2:B:1349:C:H5' | 1.98 | 0.46 |
| 2:B:1773:A:N7 | 2:B:1829:A:H1' | 2.29 | 0.46 |
| 7:P:89:GLY:HA2 | 7:P:111:GLU:C | 2.36 | 0.46 |
| 20:J:64:VAL:HG22 | 20:J:68:LYS:CD | 2.45 | 0.46 |
| 2:B:1317:G:H2' | 2:B:1318:U:H6 | 1.80 | 0.46 |
| 1:A:13:G:H2' | 1:A:14:U:H5'' | 1.97 | 0.46 |
| 2:B:2457:U:H2' | 2:B:2458:G:H5' | 1.97 | 0.46 |
| 5:D:141:ARG:HG3 | 5:D:141:ARG:O | 2.16 | 0.46 |
| 2:B:2515:C:H2' | 2:B:2516:A:H8 | 1.81 | 0.46 |
| 2:B:929:U:H1' | 9:Y:25:GLY:O | 2.15 | 0.46 |
| 2:B:1767:G:O2' | 2:B:1768:C:H5' | 2.15 | 0.46 |
| 7:P:28:LYS:HD2 | 7:P:82:SER:OG | 2.15 | 0.46 |
| 2:B:2286:G:H4' | 2:B:2287:A:O4' | 2.15 | 0.46 |
| 2:B:2683:C:O2' | 2:B:2684:U:H5' | 2.15 | 0.46 |
| 7:P:3:ILE:HG23 | 7:P:4:ILE:N | 2.30 | 0.46 |
| 2:B:1161:C:H4' | 28:R:8:GLY:O | 2.14 | 0.46 |
| 31:W:35:ILE:O | 31:W:37:VAL:HG23 | 2.16 | 0.46 |
| 2:B:2091:C:H1' | 30:Z:34:HIS:CD2 | 2.50 | 0.46 |
| 30:Z:33:LEU:CA | 30:Z:52:SER:HA | 2.37 | 0.46 |
| 3:I:126:ARG:CB | 3:I:126:ARG:NH1 | 2.79 | 0.46 |
| 9:Y:16:LEU:O | 9:Y:19:HIS:HB2 | 2.14 | 0.46 |
| 22:O:26:LEU:HD13 | 22:O:39:VAL:CG2 | 2.46 | 0.46 |
| 19:H:97:ARG:CA | 19:H:112:LYS:HD3 | 2.45 | 0.46 |
| 20:J:72:LYS:CB | 20:J:89:PHE:H | 2.28 | 0.46 |
| 10:O:48:TYR:CG | 10:O:49:ARG:N | 2.83 | 0.46 |
| 2:B:2455:G:H2' | 2:B:2456:C:H6 | 1.79 | 0.46 |
| 2:B:304:U:H2' | 2:B:305:C:C6 | 2.50 | 0.46 |
| 2:B:2190:G:H2' | 2:B:2191:A:H8 | 1.80 | 0.46 |
| 20:J:23:LYS:NZ | 20:J:142:ILE:HG23 | 2.30 | 0.46 |
| 15:2:10:LEU:O | 15:2:14:ARG:HG2 | 2.16 | 0.46 |
| 2:B:41:C:O2' | 2:B:42:A:H5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:93:G:H2' | 2:B:94:A:O4' | 2.15 | 0.46 |
| 2:B:922:C:H1' | 31:W:22:VAL:HG21 | 1.96 | 0.46 |
| 8:E:155:GLU:HB3 | 8:E:159:LEU:HD13 | 1.98 | 0.46 |
| 27:G:25:ILE:CG2 | 27:G:78:VAL:HG21 | 2.46 | 0.46 |
| 29:T:14:PRO:HA | 29:T:32:LEU:HB3 | 1.97 | 0.46 |
| 2:B:2528:U:O2' | 2:B:2529:G:H3' | 2.15 | 0.46 |
| 3:I:23:VAL:HG12 | 3:I:24:GLY:N | 2.30 | 0.46 |
| 2:B:2052:A:H4' | 5:D:148:GLN:N | 2.31 | 0.46 |
| 20:J:55:ILE:HB | 20:J:123:LYS:HB2 | 1.96 | 0.46 |
| 3:I:45:THR:HA | 3:I:48:ILE:CG2 | 2.39 | 0.46 |
| 27:G:145:ALA:O | 27:G:149:ALA:N | 2.47 | 0.46 |
| 25:U:73:ASN:HB3 | 25:U:95:PHE:CE2 | 2.49 | 0.46 |
| 8:E:146:VAL:HB | 8:E:148:ILE:HD11 | 1.97 | 0.46 |
| 14:V:3:THR:HA | 14:V:62:THR:OG1 | 2.16 | 0.46 |
| 2:B:665:U:O2' | 2:B:666:A:H5' | 2.15 | 0.46 |
| 2:B:1857:G:N2 | 2:B:1884:G:H2' | 2.31 | 0.46 |
| 2:B:1507:C:C3' | 2:B:1508:A:H4' | 2.46 | 0.46 |
| 2:B:1196:C:H2' | 2:B:1197:G:H8 | 1.77 | 0.46 |
| 2:B:1818:U:HO2' | 2:B:1819:A:P | 2.38 | 0.46 |
| 2:B:549:G:H3' | 20:J:2:LYS:HE3 | 1.97 | 0.46 |
| 16:L:135:ILE:HG23 | 16:L:136:GLU:N | 2.30 | 0.46 |
| 3:I:102:ARG:HG3 | 3:I:141:ASP:CB | 2.44 | 0.46 |
| 2:B:2233:U:H2' | 2:B:2234:G:C8 | 2.50 | 0.46 |
| 20:J:44:TYR:C | 20:J:44:TYR:CD2 | 2.88 | 0.46 |
| 28:R:6:GLN:HE21 | 28:R:7:SER:N | 2.13 | 0.46 |
| 2:B:348:A:H2' | 2:B:349:U:O4' | 2.16 | 0.46 |
| 26:F:119:LYS:HA | 26:F:121:PHE:CZ | 2.50 | 0.46 |
| 26:F:121:PHE:HA | 26:F:127:TYR:HA | 1.98 | 0.46 |
| 30:Z:53:ALA:O | 30:Z:55:GLY:N | 2.44 | 0.46 |
| 19:H:131:SER:HA | 19:H:140:ALA:O | 2.16 | 0.46 |
| 17:M:28:PHE:HB3 | 17:M:64:TRP:CE2 | 2.49 | 0.46 |
| 7:P:61:ARG:NH1 | 7:P:100:ARG:HA | 2.31 | 0.46 |
| 2:B:2598:A:H5'' | 4:C:233:GLY:O | 2.16 | 0.46 |
| 2:B:1405:U:H2' | 2:B:1406:U:H6 | 1.78 | 0.46 |
| 14:V:64:VAL:HG13 | 14:V:68:LYS:O | 2.15 | 0.46 |
| 2:B:308:G:H2' | 2:B:309:A:O4' | 2.16 | 0.46 |
| 2:B:1197:G:O2' | 2:B:1198:U:H5' | 2.16 | 0.46 |
| 2:B:155:A:H2' | 2:B:156:A:H8 | 1.79 | 0.46 |
| 2:B:1093:G:O2' | 2:B:1094:U:H5' | 2.16 | 0.46 |
| 2:B:129:C:H2' | 2:B:130:C:C6 | 2.50 | 0.46 |
| 2:B:2218:G:O2' | 2:B:2219:U:H5' | 2.16 | 0.46 |
| 26:F:8:LYS:HD3 | 26:F:9:ASP:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 5:D:97:SER:HB3 | 5:D:99:GLU:HG3 | 1.98 | 0.46 |
| 2:B:1649:G:O2' | 2:B:1650:A:H5' | 2.16 | 0.46 |
| 3:I:2:LYS:N | 3:I:2:LYS:HD2 | 2.31 | 0.46 |
| 2:B:2272:U:H5'' | 2:B:2273:A:OP1 | 2.16 | 0.46 |
| 2:B:922:C:O2' | 31:W:25:PHE:HZ | 1.99 | 0.46 |
| 27:G:29:ASN:ND2 | 27:G:77:GLY:O | 2.48 | 0.46 |
| 6:K:35:VAL:CG2 | 6:K:36:GLY:H | 2.12 | 0.46 |
| 2:B:1813:G:H1' | 4:C:49:THR:OG1 | 2.16 | 0.46 |
| 19:H:3:VAL:HB | 19:H:37:VAL:O | 2.15 | 0.46 |
| 4:C:147:PRO:HD3 | 4:C:184:GLU:HB2 | 1.97 | 0.46 |
| 6:K:72:PRO:O | 6:K:74:GLY:N | 2.48 | 0.46 |
| 2:B:1177:G:H2' | 2:B:1178:C:H6 | 1.78 | 0.46 |
| 2:B:1060:U:OP2 | 3:I:74:PRO:HA | 2.15 | 0.46 |
| 24:S:29:VAL:O | 24:S:33:LEU:HB2 | 2.16 | 0.46 |
| 20:J:56:VAL:HG12 | 20:J:57:LEU:N | 2.31 | 0.46 |
| 30:Z:59:ILE:HG23 | 30:Z:67:VAL:HG21 | 1.98 | 0.46 |
| 2:B:358:U:H6 | 2:B:358:U:O5' | 1.98 | 0.46 |
| 2:B:360:U:H2' | 2:B:361:G:N9 | 2.31 | 0.46 |
| 25:U:53:GLN:N | 25:U:54:PRO:CD | 2.78 | 0.46 |
| 2:B:289:G:H2' | 2:B:290:U:H6 | 1.77 | 0.46 |
| 17:M:108:VAL:HG13 | 17:M:112:LEU:HB3 | 1.97 | 0.46 |
| 26:F:47:LYS:HA | 26:F:50:ASP:OD1 | 2.15 | 0.46 |
| 19:H:127:GLU:CD | 19:H:127:GLU:H | 2.19 | 0.46 |
| 4:C:248:GLY:C | 4:C:249:VAL:HG22 | 2.36 | 0.46 |
| 4:C:255:LYS:C | 4:C:256:THR:HG23 | 2.35 | 0.46 |
| 2:B:2898:U:H2' | 2:B:2899:A:C8 | 2.50 | 0.46 |
| 2:B:1163:G:O2' | 2:B:1164:C:H5' | 2.16 | 0.46 |
| 2:B:904:G:H2' | 2:B:905:A:H8 | 1.81 | 0.46 |
| 2:B:12:U:O2 | 2:B:2626:C:H4' | 2.15 | 0.46 |
| 2:B:1432:G:O2' | 2:B:1433:A:H5' | 2.15 | 0.46 |
| 2:B:1557:C:H3' | 2:B:1558:C:C5' | 2.46 | 0.46 |
| 2:B:2098:U:H2' | 2:B:2099:U:O4' | 2.16 | 0.46 |
| 2:B:1559:U:H3' | 2:B:1560:G:H5' | 1.98 | 0.46 |
| 2:B:205:G:HO2' | 2:B:206:U:P | 2.38 | 0.46 |
| 2:B:2249:U:H4' | 2:B:2275:C:C5 | 2.51 | 0.46 |
| 2:B:1607:C:N4 | 2:B:1622:G:OP2 | 2.48 | 0.46 |
| 2:B:378:C:O2' | 2:B:379:G:H5' | 2.16 | 0.46 |
| 17:M:78:LEU:O | 17:M:80:VAL:HG12 | 2.15 | 0.46 |
| 2:B:2365:G:O2' | 31:W:59:PHE:CE1 | 2.69 | 0.46 |
| 31:W:19:ARG:HD3 | 31:W:36:ILE:HD11 | 1.98 | 0.46 |
| 2:B:558:U:O3' | 20:J:111:LYS:HE2 | 2.16 | 0.46 |
| 28:R:40:MET:HG2 | 28:R:48:LYS:HA | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:98:G:H1 | 14:V:14:LYS:CB | 2.18 | 0.46 |
| 5:D:8:LYS:O | 5:D:9:VAL:HB | 2.16 | 0.46 |
| 26:F:131:VAL:C | 26:F:133:GLU:H | 2.19 | 0.46 |
| 26:F:131:VAL:O | 26:F:132:ARG:HB2 | 2.16 | 0.46 |
| 28:R:2:TYR:CB | 28:R:42:ALA:HB2 | 2.38 | 0.46 |
| 30:Z:53:ALA:O | 30:Z:54:LYS:HB3 | 2.15 | 0.46 |
| 2:B:360:U:H2' | 2:B:361:G:C1' | 2.46 | 0.46 |
| 12:1:3:GLY:O | 12:1:5:ARG:N | 2.49 | 0.46 |
| 2:B:625:G:H2' | 2:B:626:A:C8 | 2.51 | 0.46 |
| 5:D:118:PHE:HZ | 5:D:123:LYS:NZ | 2.14 | 0.46 |
| 28:R:15:SER:H | 28:R:18:GLN:CG | 2.28 | 0.46 |
| 20:J:74:TYR:HB2 | 20:J:87:ALA:O | 2.15 | 0.46 |
| 11:4:36:ARG:CG | 11:4:37:GLN:H | 2.28 | 0.46 |
| 1:A:105:G:O2' | 1:A:106:G:H5' | 2.16 | 0.46 |
| 2:B:659:G:H4' | 8:E:95:LYS:HB3 | 1.96 | 0.46 |
| 1:A:89:U:O2 | 2:B:958:U:H2' | 2.16 | 0.46 |
| 2:B:1316:U:H2' | 2:B:1317:G:H8 | 1.80 | 0.46 |
| 2:B:2602:A:H4' | 2:B:2603:G:C5' | 2.45 | 0.46 |
| 24:S:88:ARG:HH21 | 24:S:88:ARG:HG3 | 1.80 | 0.46 |
| 2:B:104:A:H2' | 2:B:105:C:H6 | 1.80 | 0.46 |
| 1:A:16:G:O2' | 1:A:17:C:H5' | 2.15 | 0.46 |
| 16:L:125:LEU:H | 16:L:143:GLU:CG | 2.29 | 0.46 |
| 20:J:38:GLY:O | 20:J:43:GLU:HB2 | 2.16 | 0.46 |
| 20:J:42:ALA:O | 20:J:44:TYR:N | 2.49 | 0.46 |
| 5:D:191:GLY:O | 5:D:192:ALA:HB3 | 2.15 | 0.46 |
| 29:T:7:LEU:HD22 | 29:T:9:LYS:HE3 | 1.98 | 0.46 |
| 3:I:79:LEU:HD12 | 3:I:135:MET:SD | 2.55 | 0.46 |
| 26:F:89:THR:O | 26:F:91:ARG:CZ | 2.64 | 0.46 |
| 31:W:37:VAL:HG22 | 31:W:55:ASP:O | 2.16 | 0.46 |
| 5:D:90:PHE:N | 5:D:94:GLN:OE1 | 2.47 | 0.46 |
| 22:O:93:ASP:C | 22:O:95:SER:H | 2.18 | 0.46 |
| 2:B:358:U:H2' | 2:B:359:G:C8 | 2.50 | 0.46 |
| 9:Y:16:LEU:HD23 | 9:Y:19:HIS:CD2 | 2.51 | 0.46 |
| 9:Y:18:LYS:O | 9:Y:22:THR:HG23 | 2.16 | 0.46 |
| 6:K:119:ALA:HB3 | 6:K:120:PRO:CD | 2.46 | 0.46 |
| 20:J:99:ARG:HA | 20:J:102:GLU:HB2 | 1.97 | 0.46 |
| 2:B:826:U:H2' | 2:B:828:U:O4' | 2.16 | 0.46 |
| 2:B:275:C:O2 | 2:B:276:U:H1' | 2.16 | 0.46 |
| 2:B:156:A:O2' | 2:B:157:C:H5' | 2.16 | 0.46 |
| 2:B:673:C:H2' | 2:B:674:G:H5' | 1.98 | 0.46 |
| 2:B:337:C:H2' | 2:B:338:G:O4' | 2.16 | 0.46 |
| 2:B:1495:A:O2' | 2:B:1496:A:H5' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:1958:C:O2' | 2:B:1959:G:H5' | 2.14 | 0.46 |
| 2:B:1190:G:OP1 | 16:L:33:ARG:N | 2.48 | 0.46 |
| 16:L:19:LEU:O | 16:L:21:ARG:HG2 | 2.15 | 0.46 |
| 30:Z:18:ARG:HA | 30:Z:23:ASN:O | 2.15 | 0.46 |
| 17:M:65:ILE:HD12 | 17:M:65:ILE:N | 2.30 | 0.46 |
| 2:B:500:G:N2 | 2:B:502:A:H3' | 2.30 | 0.46 |
| 4:C:161:VAL:HG12 | 4:C:162:GLN:N | 2.31 | 0.46 |
| 2:B:467:G:O2' | 2:B:468:G:H5' | 2.16 | 0.46 |
| 2:B:2686:G:H2' | 2:B:2687:U:C6 | 2.51 | 0.46 |
| 7:P:36:LYS:C | 7:P:37:LYS:HD3 | 2.36 | 0.46 |
| 2:B:1099:G:O4' | 3:I:3:LYS:O | 2.33 | 0.46 |
| 27:G:18:ILE:HA | 27:G:22:VAL:O | 2.16 | 0.46 |
| 26:F:32:LYS:HZ2 | 26:F:156:THR:HG21 | 1.81 | 0.46 |
| 2:B:2654:A:N1 | 2:B:2665:A:H5'' | 2.30 | 0.46 |
| 19:H:21:VAL:HG22 | 19:H:22:LYS:N | 2.31 | 0.46 |
| 7:P:51:ASN:O | 7:P:52:ARG:HD3 | 2.16 | 0.46 |
| 30:Z:2:SER:O | 30:Z:4:VAL:HG22 | 2.16 | 0.46 |
| 2:B:1203:U:C4' | 16:L:3:LEU:HD12 | 2.44 | 0.46 |
| 21:N:28:LEU:O | 21:N:32:GLU:HA | 2.15 | 0.46 |
| 28:R:15:SER:OG | 28:R:18:GLN:HG2 | 2.16 | 0.46 |
| 2:B:454:A:H4' | 2:B:455:C:OP2 | 2.16 | 0.46 |
| 20:J:97:PRO:HD2 | 20:J:98:GLU:OE2 | 2.16 | 0.46 |
| 2:B:1047:G:H1' | 2:B:1110:G:C2 | 2.51 | 0.46 |
| 2:B:370:G:HO2' | 2:B:423:A:H3' | 1.78 | 0.46 |
| 2:B:1820:U:H3 | 4:C:197:ALA:HA | 1.81 | 0.46 |
| 2:B:2103:C:H5'' | 2:B:2104:C:OP2 | 2.16 | 0.46 |
| 2:B:1827:U:H2' | 2:B:1828:G:H5' | 1.97 | 0.46 |
| 1:A:116:G:H4' | 22:O:54:VAL:CG2 | 2.46 | 0.46 |
| 20:J:23:LYS:HZ1 | 20:J:142:ILE:HG12 | 1.81 | 0.46 |
| 22:O:58:ILE:O | 22:O:62:LEU:HD23 | 2.15 | 0.46 |
| 2:B:2446:G:H2' | 2:B:2447:G:H5'' | 1.97 | 0.46 |
| 4:C:2:VAL:HG23 | 4:C:3:VAL:N | 2.31 | 0.46 |
| 2:B:2637:U:OP1 | 5:D:83:ARG:HD3 | 2.15 | 0.46 |
| 4:C:270:ARG:NH1 | 4:C:270:ARG:HB3 | 2.31 | 0.46 |
| 2:B:72:U:O2' | 2:B:73:A:H5' | 2.16 | 0.46 |
| 2:B:178:G:O2' | 2:B:179:C:H5' | 2.16 | 0.46 |
| 10:O:56:LYS:O | 10:O:56:LYS:HD3 | 2.15 | 0.46 |
| 2:B:2864:G:H2' | 2:B:2865:U:C6 | 2.51 | 0.46 |
| 2:B:1099:G:N7 | 3:I:3:LYS:HD3 | 2.30 | 0.46 |
| 25:U:86:PHE:HB2 | 25:U:92:VAL:HB | 1.98 | 0.46 |
| 27:G:8:VAL:HG21 | 27:G:49:LEU:CB | 2.38 | 0.46 |
| 28:R:66:HIS:CG | 28:R:94:THR:HG22 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:Q:4:LYS:CE | 23:Q:7:VAL:HG22 | 2.33 | 0.46 |
| 4:C:166:ARG:NH2 | 4:C:166:ARG:HB2 | 2.31 | 0.46 |
| 3:I:78:LEU:HD23 | 3:I:81:LYS:HE2 | 1.97 | 0.46 |
| 26:F:127:TYR:HB3 | 26:F:155:ILE:HD13 | 1.98 | 0.46 |
| 2:B:1439:A:N7 | 2:B:1440:U:C6 | 2.85 | 0.46 |
| 17:M:101:VAL:HG13 | 17:M:101:VAL:O | 2.15 | 0.46 |
| 12:1:7:LYS:HD3 | 12:1:23:THR:HG22 | 1.97 | 0.46 |
| 2:B:819:A:OP2 | 2:B:1187:G:N2 | 2.47 | 0.46 |
| 22:O:30:ARG:HG2 | 22:O:102:ARG:NH1 | 2.31 | 0.46 |
| 2:B:840:C:H2' | 2:B:841:G:C8 | 2.50 | 0.46 |
| 2:B:2299:U:H2' | 2:B:2300:C:C6 | 2.51 | 0.46 |
| 2:B:935:C:H2' | 2:B:936:A:H8 | 1.81 | 0.46 |
| 20:J:23:LYS:HZ2 | 20:J:142:ILE:HG23 | 1.81 | 0.46 |
| 19:H:57:LYS:HG3 | 19:H:58:LEU:N | 2.31 | 0.46 |
| 5:D:46:ARG:HB3 | 5:D:84:LEU:HD12 | 1.98 | 0.46 |
| 2:B:57:C:H2' | 2:B:58:G:C8 | 2.51 | 0.46 |
| 2:B:464:U:H2' | 2:B:465:G:O4' | 2.16 | 0.46 |
| 2:B:2266:A:N3 | 2:B:2272:U:H5 | 2.14 | 0.45 |
| 11:4:35:GLN:HE21 | 11:4:35:GLN:HB2 | 1.56 | 0.45 |
| 21:N:61:ALA:C | 21:N:63:ARG:N | 2.68 | 0.45 |
| 2:B:1551:A:C3' | 2:B:1552:A:H5'' | 2.46 | 0.45 |
| 20:J:124:VAL:HG23 | 20:J:125:TYR:H | 1.81 | 0.45 |
| 29:T:20:ALA:O | 29:T:24:MET:HB2 | 2.15 | 0.45 |
| 8:E:160:ALA:C | 8:E:162:ARG:H | 2.20 | 0.45 |
| 23:Q:24:TYR:CG | 23:Q:25:GLY:N | 2.84 | 0.45 |
| 5:D:68:PHE:HB3 | 5:D:73:VAL:CG2 | 2.42 | 0.45 |
| 2:B:845:A:N1 | 2:B:847:U:H1' | 2.31 | 0.45 |
| 16:L:57:LEU:C | 16:L:59:ARG:H | 2.18 | 0.45 |
| 2:B:263:G:H2' | 2:B:264:C:C6 | 2.51 | 0.45 |
| 2:B:2400:G:C2' | 2:B:2401:U:H5' | 2.46 | 0.45 |
| 2:B:2026:U:C2 | 2:B:2027:G:C8 | 3.05 | 0.45 |
| 27:G:106:LEU:N | 27:G:106:LEU:HD23 | 2.31 | 0.45 |
| 2:B:2408:U:O2' | 2:B:2409:G:H5' | 2.15 | 0.45 |
| 2:B:624:C:O2' | 2:B:657:U:H5'' | 2.16 | 0.45 |
| 5:D:4:LEU:HD21 | 5:D:100:LEU:CB | 2.45 | 0.45 |
| 2:B:1106:G:H2' | 2:B:1107:G:C8 | 2.50 | 0.45 |
| 2:B:781:A:OP1 | 4:C:216:ARG:NH2 | 2.49 | 0.45 |
| 17:M:82:MET:O | 17:M:84:LYS:HG2 | 2.17 | 0.45 |
| 2:B:1248:G:OP1 | 23:Q:1:ALA:HB3 | 2.16 | 0.45 |
| 2:B:1743:G:H8 | 2:B:1743:G:O5' | 1.99 | 0.45 |
| 14:V:51:GLN:HB2 | 14:V:57:TYR:OH | 2.17 | 0.45 |
| 29:T:48:GLN:HA | 29:T:48:GLN:NE2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:2306:C:H3' | 2:B:2307:G:C5' | 2.35 | 0.45 |
| 18:X:15:ASN:O | 18:X:19:LEU:HD13 | 2.16 | 0.45 |
| 26:F:110:ILE:HA | 26:F:111:ARG:NE | 2.31 | 0.45 |
| 26:F:35:LEU:HD23 | 26:F:153:ILE:HG12 | 1.99 | 0.45 |
| 26:F:62:GLN:HE21 | 26:F:91:ARG:HH11 | 1.64 | 0.45 |
| 2:B:675:A:OP1 | 8:E:60:TRP:CZ2 | 2.69 | 0.45 |
| 30:Z:6:GLN:NE2 | 30:Z:50:ARG:H | 2.07 | 0.45 |
| 2:B:1081:U:C5' | 3:I:126:ARG:NH1 | 2.76 | 0.45 |
| 3:I:100:ILE:HG23 | 3:I:104:GLN:OE1 | 2.17 | 0.45 |
| 13:3:7:ARG:HG3 | 13:3:7:ARG:HH11 | 1.82 | 0.45 |
| 2:B:2195:U:O2' | 2:B:2196:C:H5' | 2.16 | 0.45 |
| 2:B:950:G:H2' | 2:B:951:C:H6 | 1.81 | 0.45 |
| 29:T:61:LEU:HD12 | 29:T:62:VAL:O | 2.17 | 0.45 |
| 20:J:114:LEU:O | 20:J:118:MET:HE2 | 2.15 | 0.45 |
| 2:B:1774:C:H2' | 2:B:1774:C:O2 | 2.16 | 0.45 |
| 13:3:28:LEU:O | 13:3:28:LEU:HG | 2.16 | 0.45 |
| 5:D:105:LYS:H | 5:D:106:LYS:HZ3 | 1.65 | 0.45 |
| 27:G:36:LEU:CD2 | 27:G:36:LEU:H | 2.28 | 0.45 |
| 27:G:8:VAL:CG1 | 27:G:49:LEU:H | 2.13 | 0.45 |
| 2:B:558:U:H5'' | 20:J:111:LYS:HD3 | 1.98 | 0.45 |
| 2:B:351:C:H2' | 2:B:352:A:H8 | 1.81 | 0.45 |
| 11:4:8:LYS:HG2 | 11:4:9:LYS:HD3 | 1.99 | 0.45 |
| 2:B:1161:C:H1' | 28:R:9:GLY:HA3 | 1.97 | 0.45 |
| 3:I:27:LEU:HB2 | 3:I:32:VAL:HG21 | 1.97 | 0.45 |
| 20:J:16:TYR:CD2 | 20:J:140:LEU:HD12 | 2.50 | 0.45 |
| 2:B:139:U:C2 | 29:T:1:MET:HB3 | 2.52 | 0.45 |
| 9:Y:16:LEU:CD2 | 9:Y:16:LEU:H | 2.23 | 0.45 |
| 2:B:851:C:O4' | 9:Y:46:MET:HG3 | 2.17 | 0.45 |
| 19:H:110:VAL:HG13 | 19:H:110:VAL:O | 2.17 | 0.45 |
| 27:G:95:ALA:HA | 27:G:104:LEU:HD23 | 1.98 | 0.45 |
| 6:K:75:SER:HB2 | 7:P:73:PHE:HA | 1.98 | 0.45 |
| 2:B:2820:A:OP1 | 21:N:4:ARG:HA | 2.16 | 0.45 |
| 17:M:108:VAL:HG21 | 17:M:112:LEU:HD12 | 1.97 | 0.45 |
| 2:B:972:A:C3' | 2:B:973:A:H5'' | 2.42 | 0.45 |
| 2:B:1843:C:H2' | 2:B:1844:C:H6 | 1.80 | 0.45 |
| 2:B:1693:U:O2' | 4:C:13:ARG:NH2 | 2.46 | 0.45 |
| 2:B:2873:A:O4' | 21:N:6:SER:HB3 | 2.17 | 0.45 |
| 24:S:108:SER:OG | 24:S:109:ASP:N | 2.49 | 0.45 |
| 2:B:1152:C:O2' | 2:B:1153:C:H5' | 2.15 | 0.45 |
| 2:B:1636:U:H2' | 2:B:1637:A:C8 | 2.52 | 0.45 |
| 2:B:1099:G:O5' | 3:I:3:LYS:CA | 2.64 | 0.45 |
| 19:H:4:ILE:HG13 | 19:H:18:GLN:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:I:57:VAL:HG23 | 3:I:71:LYS:HZ1 | 1.80 | 0.45 |
| 2:B:1454:C:C1' | 21:N:60:VAL:HG13 | 2.42 | 0.45 |
| 24:S:28:LYS:HD3 | 24:S:69:LEU:O | 2.16 | 0.45 |
| 26:F:108:PRO:O | 26:F:110:ILE:HG23 | 2.17 | 0.45 |
| 26:F:116:LEU:HD12 | 26:F:117:SER:N | 2.32 | 0.45 |
| 1:A:6:G:H2' | 1:A:7:G:H8 | 1.81 | 0.45 |
| 2:B:1103:A:H3' | 2:B:1104:C:C6 | 2.50 | 0.45 |
| 25:U:73:ASN:C | 25:U:75:ALA:H | 2.20 | 0.45 |
| 3:I:138:VAL:HG12 | 3:I:139:VAL:N | 2.31 | 0.45 |
| 12:1:47:ILE:HD12 | 12:1:47:ILE:H | 1.81 | 0.45 |
| 11:4:16:ILE:HG12 | 11:4:25:VAL:CG2 | 2.46 | 0.45 |
| 2:B:2228:G:H2' | 2:B:2229:U:C6 | 2.52 | 0.45 |
| 2:B:1276:A:O2' | 2:B:1277:G:H5' | 2.17 | 0.45 |
| 2:B:2691:C:H2' | 2:B:2692:G:H8 | 1.82 | 0.45 |
| 26:F:37:MET:SD | 26:F:56:LEU:HD23 | 2.56 | 0.45 |
| 2:B:2540:C:H2' | 2:B:2541:A:C8 | 2.52 | 0.45 |
| 2:B:103:A:H3' | 2:B:104:A:H8 | 1.82 | 0.45 |
| 2:B:2747:G:H8 | 2:B:2747:G:O5' | 2.00 | 0.45 |
| 30:Z:49:LEU:H | 30:Z:49:LEU:HD12 | 1.81 | 0.45 |
| 23:Q:34:ALA:O | 23:Q:38:VAL:HG23 | 2.16 | 0.45 |
| 18:X:39:GLN:CB | 18:X:42:LEU:HD22 | 2.47 | 0.45 |
| 19:H:90:LEU:HD22 | 19:H:122:LEU:O | 2.16 | 0.45 |
| 29:T:11:LEU:HD11 | 29:T:46:ALA:CB | 2.46 | 0.45 |
| 29:T:85:VAL:C | 29:T:86:THR:HG23 | 2.36 | 0.45 |
| 26:F:91:ARG:C | 26:F:95:MET:HB2 | 2.37 | 0.45 |
| 11:4:19:ARG:C | 11:4:21:GLY:N | 2.70 | 0.45 |
| 2:B:138:U:H1' | 29:T:2:ILE:HG23 | 1.97 | 0.45 |
| 2:B:637:A:C5' | 16:L:112:LEU:HD22 | 2.44 | 0.45 |
| 16:L:79:LEU:HD12 | 16:L:114:GLY:H | 1.81 | 0.45 |
| 3:I:129:GLU:CB | 3:I:133:ARG:HH12 | 2.29 | 0.45 |
| 3:I:96:LYS:HD3 | 3:I:138:VAL:HG21 | 1.98 | 0.45 |
| 2:B:580:U:O2' | 2:B:581:C:H5' | 2.17 | 0.45 |
| 26:F:134:GLN:O | 26:F:136:ILE:N | 2.48 | 0.45 |
| 17:M:57:VAL:O | 17:M:59:ARG:N | 2.49 | 0.45 |
| 2:B:528:A:H2 | 2:B:2043:C:H4' | 1.82 | 0.45 |
| 2:B:1150:C:H2' | 2:B:1151:A:H8 | 1.81 | 0.45 |
| 2:B:2109:U:C4 | 2:B:2180:U:H2' | 2.52 | 0.45 |
| 30:Z:41:GLU:O | 30:Z:44:LYS:HD2 | 2.17 | 0.45 |
| 11:4:15:LYS:O | 11:4:16:ILE:CB | 2.65 | 0.45 |
| 2:B:154:U:H2' | 2:B:155:A:C8 | 2.52 | 0.45 |
| 2:B:2299:U:H2' | 2:B:2300:C:H6 | 1.82 | 0.45 |
| 2:B:234:U:H2' | 2:B:235:U:H6 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:707:G:O2' | 2:B:708:G:H5' | 2.17 | 0.45 |
| 2:B:770:G:H1' | 2:B:1379:U:C4 | 2.52 | 0.45 |
| 16:L:131:ALA:O | 16:L:135:ILE:HG22 | 2.16 | 0.45 |
| 2:B:1395:A:H4' | 2:B:1397:U:C5 | 2.52 | 0.45 |
| 1:A:82:U:O2' | 1:A:83:G:H5' | 2.16 | 0.45 |
| 2:B:179:C:H2' | 2:B:180:G:O4' | 2.16 | 0.45 |
| 2:B:215:G:H4' | 2:B:216:A:OP1 | 2.15 | 0.45 |
| 2:B:1863:G:H2' | 2:B:1864:U:O4' | 2.16 | 0.45 |
| 2:B:1052:C:H2' | 2:B:1053:C:C6 | 2.52 | 0.45 |
| 27:G:58:ALA:C | 27:G:60:GLY:H | 2.19 | 0.45 |
| 19:H:94:ILE:HG13 | 19:H:98:ASP:HB3 | 1.99 | 0.45 |
| 29:T:16:VAL:HG12 | 29:T:22:THR:HG22 | 1.99 | 0.45 |
| 21:N:75:ILE:HD12 | 21:N:79:LEU:HD12 | 1.98 | 0.45 |
| 1:A:43:C:H2' | 1:A:44:G:H5'' | 1.97 | 0.45 |
| 26:F:1:ALA:O | 26:F:4:HIS:HB3 | 2.16 | 0.45 |
| 26:F:62:GLN:CG | 26:F:91:ARG:HH11 | 2.21 | 0.45 |
| 19:H:9:VAL:CG1 | 19:H:12:LEU:HG | 2.46 | 0.45 |
| 16:L:3:LEU:O | 16:L:5:THR:HG23 | 2.16 | 0.45 |
| 19:H:73:ASN:OD1 | 19:H:142:VAL:HA | 2.16 | 0.45 |
| 17:M:35:ALA:HB3 | 17:M:100:LYS:H | 1.82 | 0.45 |
| 20:J:96:ARG:CZ | 20:J:99:ARG:HD2 | 2.47 | 0.45 |
| 2:B:712:G:H2' | 2:B:713:G:O4' | 2.17 | 0.45 |
| 22:O:56:LYS:HG2 | 22:O:60:GLU:OE1 | 2.15 | 0.45 |
| 30:Z:65:ASP:O | 30:Z:69:ALA:N | 2.49 | 0.45 |
| 23:Q:9:ALA:C | 23:Q:11:ALA:N | 2.70 | 0.45 |
| 20:J:59:ALA:C | 20:J:61:LYS:N | 2.69 | 0.45 |
| 18:X:23:ARG:HB3 | 18:X:27:ASN:OD1 | 2.17 | 0.45 |
| 2:B:2405:G:H1' | 2:B:2412:A:H61 | 1.82 | 0.45 |
| 2:B:863:A:H2' | 2:B:864:G:C8 | 2.51 | 0.45 |
| 2:B:1491:G:H5' | 4:C:97:ASP:OD1 | 2.17 | 0.45 |
| 21:N:41:ALA:C | 21:N:43:GLU:H | 2.20 | 0.45 |
| 30:Z:18:ARG:NH1 | 30:Z:24:ALA:HB2 | 2.31 | 0.45 |
| 2:B:129:C:H2' | 2:B:130:C:H6 | 1.82 | 0.45 |
| 2:B:1365:A:H2' | 2:B:1365:A:N3 | 2.32 | 0.45 |
| 2:B:2614:A:O4' | 10:O:1:ALA:HB3 | 2.17 | 0.45 |
| 25:U:85:ARG:NH1 | 25:U:86:PHE:N | 2.65 | 0.45 |
| 18:X:31:GLN:HA | 18:X:36:GLN:OE1 | 2.17 | 0.45 |
| 29:T:29:THR:H | 29:T:91:GLN:NE2 | 2.07 | 0.45 |
| 8:E:28:VAL:O | 8:E:32:VAL:HG13 | 2.16 | 0.45 |
| 26:F:111:ARG:NH2 | 26:F:113:PHE:HB2 | 2.32 | 0.45 |
| 2:B:1444:G:H2' | 2:B:1445:G:H8 | 1.82 | 0.45 |
| 20:J:81:ILE:HG12 | 20:J:82:GLY:N | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 16:L:6:LEU:HD23 | 16:L:6:LEU:N | 2.24 | 0.45 |
| 1:A:52:A:H2' | 1:A:53:A:H5' | 1.99 | 0.45 |
| 12:1:12:SER:HB2 | 12:1:48:TYR:CE1 | 2.52 | 0.45 |
| 2:B:850:U:O2' | 9:Y:22:THR:HG22 | 2.17 | 0.45 |
| 2:B:1616:A:H4' | 2:B:1617:C:OP2 | 2.17 | 0.45 |
| 19:H:126:GLY:N | 19:H:146:VAL:HB | 2.31 | 0.45 |
| 6:K:113:MET:HE1 | 6:K:116:ILE:HD11 | 1.98 | 0.45 |
| 2:B:1045:C:O2 | 2:B:1047:G:N2 | 2.49 | 0.45 |
| 13:3:49:VAL:CG2 | 13:3:54:LEU:HD13 | 2.46 | 0.45 |
| 2:B:1856:U:C2' | 2:B:1857:G:H5' | 2.43 | 0.45 |
| 2:B:64:A:H2' | 2:B:65:U:H6 | 1.81 | 0.45 |
| 22:O:35:ILE:HG13 | 22:O:71:ALA:HB1 | 1.98 | 0.45 |
| 2:B:840:C:H2' | 2:B:841:G:H8 | 1.81 | 0.45 |
| 22:O:74:VAL:O | 22:O:77:ALA:HB3 | 2.17 | 0.45 |
| 2:B:320:A:C2 | 8:E:163:ASN:HB3 | 2.52 | 0.45 |
| 1:A:13:G:C2' | 1:A:14:U:H5'' | 2.47 | 0.45 |
| 2:B:26:G:H1' | 2:B:514:A:H61 | 1.81 | 0.45 |
| 3:I:89:SER:HA | 3:I:97:VAL:HG11 | 1.99 | 0.45 |
| 11:4:1:MET:HE1 | 11:4:24:ARG:NH2 | 2.31 | 0.45 |
| 2:B:807:U:H2' | 2:B:808:G:H8 | 1.82 | 0.45 |
| 17:M:54:THR:O | 17:M:56:ALA:N | 2.48 | 0.45 |
| 2:B:1098:A:C3' | 3:I:3:LYS:C | 2.85 | 0.45 |
| 2:B:2354:C:H4' | 31:W:31:LEU:CD2 | 2.45 | 0.45 |
| 25:U:85:ARG:CD | 25:U:86:PHE:H | 2.08 | 0.45 |
| 2:B:558:U:O2' | 2:B:559:G:H5' | 2.17 | 0.45 |
| 23:Q:59:LEU:HD13 | 23:Q:59:LEU:C | 2.37 | 0.45 |
| 19:H:90:LEU:HD13 | 19:H:122:LEU:O | 2.15 | 0.45 |
| 3:I:49:GLU:HB3 | 3:I:52:LEU:HD12 | 1.99 | 0.45 |
| 26:F:127:TYR:HB2 | 26:F:155:ILE:HB | 1.98 | 0.45 |
| 26:F:7:TYR:OH | 26:F:29:ARG:HG3 | 2.17 | 0.45 |
| 26:F:7:TYR:HA | 26:F:11:VAL:HG23 | 1.99 | 0.45 |
| 2:B:1338:G:C4' | 29:T:18:GLU:HG3 | 2.42 | 0.45 |
| 2:B:2143:C:H2' | 2:B:2144:G:C4' | 2.46 | 0.45 |
| 27:G:148:ARG:HD3 | 27:G:152:ARG:CZ | 2.46 | 0.45 |
| 1:A:42:C:C6 | 26:F:65:LEU:HD22 | 2.52 | 0.45 |
| 4:C:157:ALA:HB1 | 4:C:196:ASN:HB3 | 1.99 | 0.45 |
| 2:B:2360:G:P | 13:3:50:SER:HB3 | 2.57 | 0.45 |
| 2:B:2648:G:H2' | 2:B:2649:C:C6 | 2.52 | 0.45 |
| 2:B:898:C:O2' | 2:B:899:A:H5'' | 2.17 | 0.45 |
| 14:V:80:HIS:CG | 14:V:83:LYS:HB2 | 2.52 | 0.45 |
| 5:D:125:TRP:CE2 | 5:D:160:LYS:HB3 | 2.51 | 0.45 |
| 8:E:150:THR:OG1 | 8:E:151:GLY:N | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:B:1316:U:H2' | 2:B:1317:G:C8 | 2.51 | 0.45 |
| 2:B:1317:G:H2' | 2:B:1318:U:C6 | 2.52 | 0.45 |
| 2:B:336:C:O2' | 2:B:337:C:H5' | 2.17 | 0.45 |
| 27:G:154:GLU:O | 27:G:156:TYR:N | 2.47 | 0.45 |
| 2:B:2708:G:O2' | 2:B:2709:G:H5' | 2.16 | 0.45 |
| 5:D:4:LEU:HD21 | 5:D:100:LEU:HB3 | 1.99 | 0.45 |
| 5:D:46:ARG:HH12 | 5:D:85:ALA:HA | 1.82 | 0.45 |
| 2:B:1258:U:H2' | 2:B:1259:G:H8 | 1.82 | 0.45 |
| 2:B:1339:G:H21 | 2:B:1603:A:H1' | 1.81 | 0.45 |
| 2:B:2843:G:O2' | 2:B:2844:G:H5' | 2.17 | 0.45 |
| 27:G:42:VAL:HB | 27:G:51:PHE:CD1 | 2.52 | 0.45 |
| 26:F:7:TYR:O | 26:F:11:VAL:HB | 2.15 | 0.45 |
| 8:E:149:ILE:O | 8:E:188:MET:HA | 2.17 | 0.45 |
| 13:3:54:LEU:O | 13:3:58:ILE:HG13 | 2.17 | 0.45 |
| 2:B:1745:A:H2' | 2:B:1746:A:C8 | 2.52 | 0.45 |
| 2:B:1946:U:H2' | 2:B:1947:C:C6 | 2.51 | 0.45 |
| 2:B:2691:C:O2' | 2:B:2692:G:H5' | 2.16 | 0.45 |
| 2:B:523:C:H4' | 2:B:540:C:O2 | 2.17 | 0.45 |
| 2:B:1260:A:O2' | 2:B:1261:C:H5' | 2.16 | 0.45 |
| 2:B:2096:C:H2' | 2:B:2097:A:C8 | 2.52 | 0.45 |
| 2:B:807:U:H2' | 2:B:808:G:C8 | 2.52 | 0.45 |
| 3:I:70:THR:HG23 | 3:I:70:THR:O | 2.16 | 0.45 |
| 20:J:95:ARG:HD3 | 20:J:95:ARG:O | 2.17 | 0.45 |
| 2:B:1210:G:N3 | 2:B:1212:G:N2 | 2.65 | 0.45 |
| 2:B:1482:G:H2' | 2:B:1483:G:H8 | 1.82 | 0.45 |
| 2:B:1545:A:H2' | 2:B:1546:G:O4' | 2.17 | 0.45 |
| 2:B:922:C:H2' | 2:B:923:G:H8 | 1.82 | 0.45 |
| 26:F:79:ARG:CZ | 26:F:82:TYR:HE2 | 2.30 | 0.45 |
| 8:E:40:ARG:HH21 | 8:E:92:HIS:HE2 | 1.64 | 0.45 |
| 2:B:283:G:H3' | 2:B:284:U:C5' | 2.46 | 0.45 |
| 17:M:69:PRO:HG2 | 17:M:70:ASP:H | 1.81 | 0.45 |
| 19:H:9:VAL:HB | 19:H:13:GLY:CA | 2.45 | 0.45 |
| 2:B:675:A:OP1 | 8:E:60:TRP:HZ2 | 2.00 | 0.45 |
| 8:E:60:TRP:O | 8:E:61:ARG:CB | 2.59 | 0.45 |
| 30:Z:7:VAL:HG13 | 30:Z:8:THR:CG2 | 2.41 | 0.45 |
| 12:1:6:GLU:HB2 | 12:1:52:LYS:CE | 2.47 | 0.45 |
| 5:D:69:ALA:HA | 5:D:73:VAL:HB | 1.98 | 0.45 |
| 6:K:78:ARG:HH12 | 7:P:70:GLU:CD | 2.21 | 0.45 |
| 22:O:66:GLY:HA3 | 22:O:102:ARG:NH2 | 2.32 | 0.45 |
| 2:B:299:A:N6 | 2:B:322:A:H1' | 2.32 | 0.45 |
| 2:B:1633:G:O2' | 2:B:1634:A:H5'' | 2.17 | 0.45 |
| 2:B:708:G:H2' | 2:B:709:U:C6 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:770:G:H5'' | 15:2:10:LEU:HD13 | 1.98 | 0.45 |
| 2:B:2626:C:O2' | 2:B:2627:G:H5' | 2.17 | 0.45 |
| 2:B:1657:U:O2' | 5:D:138:LEU:HD12 | 2.17 | 0.45 |
| 2:B:98:G:C3' | 2:B:99:U:H5'' | 2.47 | 0.45 |
| 2:B:1092:C:C2' | 2:B:1093:G:H5' | 2.47 | 0.45 |
| 23:Q:15:LYS:O | 23:Q:18:LYS:HB3 | 2.17 | 0.45 |
| 2:B:2791:G:H2' | 2:B:2792:A:O4' | 2.17 | 0.45 |
| 2:B:1754:A:OP1 | 7:P:93:LYS:HD3 | 2.17 | 0.45 |
| 2:B:1805:A:H5'' | 4:C:247:TRP:CE2 | 2.51 | 0.45 |
| 1:A:64:G:O2' | 1:A:65:U:H5' | 2.17 | 0.45 |
| 31:W:28:GLU:HB2 | 31:W:31:LEU:HD21 | 1.98 | 0.44 |
| 31:W:33:GLY:O | 31:W:34:SER:HB2 | 2.17 | 0.44 |
| 20:J:6:ALA:CB | 20:J:45:THR:HG21 | 2.47 | 0.44 |
| 2:B:1553:A:H2' | 2:B:1555:G:N7 | 2.32 | 0.44 |
| 15:2:21:ARG:HH21 | 15:2:43:THR:HG22 | 1.83 | 0.44 |
| 9:Y:28:LEU:CD1 | 9:Y:54:VAL:HG12 | 2.47 | 0.44 |
| 25:U:81:ARG:HB2 | 25:U:96:LYS:HG3 | 2.00 | 0.44 |
| 12:1:8:ILE:HG13 | 12:1:51:ALA:HA | 1.98 | 0.44 |
| 8:E:134:LEU:HD21 | 8:E:161:ALA:HB2 | 1.99 | 0.44 |
| 14:V:62:THR:CG2 | 14:V:71:LYS:HG2 | 2.45 | 0.44 |
| 4:C:196:ASN:O | 4:C:197:ALA:HB3 | 2.17 | 0.44 |
| 2:B:1410:G:H2' | 2:B:1411:U:C6 | 2.53 | 0.44 |
| 6:K:87:LEU:HB2 | 6:K:93:GLN:O | 2.16 | 0.44 |
| 2:B:1744:A:H2' | 2:B:1745:A:C8 | 2.52 | 0.44 |
| 1:A:88:C:H2' | 1:A:89:U:C5 | 2.53 | 0.44 |
| 2:B:834:G:O2' | 2:B:835:C:H5' | 2.17 | 0.44 |
| 6:K:79:PHE:O | 6:K:81:GLY:N | 2.50 | 0.44 |
| 2:B:605:G:H1' | 2:B:657:U:H1' | 1.99 | 0.44 |
| 2:B:2412:A:H2' | 2:B:2413:G:O4' | 2.17 | 0.44 |
| 2:B:598:U:H2' | 2:B:599:A:C8 | 2.52 | 0.44 |
| 1:A:76:G:O2' | 1:A:77:U:H5' | 2.16 | 0.44 |
| 2:B:1210:G:OP1 | 2:B:1212:G:H5' | 2.17 | 0.44 |
| 2:B:1544:A:H2' | 2:B:1545:A:C8 | 2.53 | 0.44 |
| 1:A:73:A:H2' | 1:A:73:A:N3 | 2.31 | 0.44 |
| 2:B:2018:G:H2' | 2:B:2019:A:C8 | 2.52 | 0.44 |
| 5:D:20:VAL:HG22 | 6:K:72:PRO:HB3 | 2.00 | 0.44 |
| 2:B:1181:U:O2' | 2:B:1182:G:H5' | 2.17 | 0.44 |
| 26:F:12:VAL:HG13 | 26:F:27:VAL:HG11 | 1.99 | 0.44 |
| 26:F:3:LEU:HD13 | 26:F:3:LEU:O | 2.16 | 0.44 |
| 19:H:49:ALA:HB3 | 19:H:50:ARG:CZ | 2.46 | 0.44 |
| 2:B:144:A:H2' | 2:B:145:C:C6 | 2.51 | 0.44 |
| 22:O:15:ARG:NH2 | 22:O:95:SER:HB3 | 2.22 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:359:G:H2' | 2:B:359:G:N3 | 2.31 | 0.44 |
| 2:B:141:G:N1 | 29:T:2:ILE:HG21 | 2.32 | 0.44 |
| 2:B:1324:G:H1' | 2:B:1616:A:C6 | 2.50 | 0.44 |
| 12:1:8:ILE:HG12 | 12:1:52:LYS:HG3 | 1.99 | 0.44 |
| 26:F:134:GLN:NE2 | 26:F:149:ARG:HB2 | 2.28 | 0.44 |
| 4:C:203:VAL:O | 4:C:205:GLY:N | 2.50 | 0.44 |
| 2:B:1229:C:H2' | 2:B:1230:A:H8 | 1.82 | 0.44 |
| 2:B:825:A:O2' | 16:L:54:GLN:NE2 | 2.50 | 0.44 |
| 22:O:94:ARG:HH21 | 22:O:94:ARG:HG2 | 1.82 | 0.44 |
| 24:S:81:SER:CA | 24:S:99:ARG:HA | 2.46 | 0.44 |
| 21:N:11:ASN:O | 21:N:12:ARG:HB2 | 2.16 | 0.44 |
| 2:B:6:A:H2' | 2:B:7:G:H8 | 1.83 | 0.44 |
| 2:B:526:A:H62 | 2:B:2626:C:H4' | 1.82 | 0.44 |
| 2:B:806:C:O2' | 2:B:807:U:H5' | 2.17 | 0.44 |
| 2:B:1760:C:H2' | 2:B:1761:C:O4' | 2.17 | 0.44 |
| 2:B:579:G:H4' | 2:B:2017:U:H2' | 1.99 | 0.44 |
| 2:B:907:G:C2' | 2:B:908:C:H5' | 2.47 | 0.44 |
| 2:B:34:U:H4' | 2:B:35:G:OP2 | 2.16 | 0.44 |
| 31:W:23:LYS:HD2 | 31:W:24:ARG:HB3 | 1.99 | 0.44 |
| 4:C:116:GLN:HG2 | 4:C:117:SER:N | 2.32 | 0.44 |
| 19:H:94:ILE:HG22 | 19:H:122:LEU:HB2 | 1.99 | 0.44 |
| 14:V:28:ALA:HB1 | 14:V:89:ILE:O | 2.17 | 0.44 |
| 4:C:79:ARG:HD2 | 4:C:81:GLU:CG | 2.47 | 0.44 |
| 8:E:29:HIS:CA | 8:E:32:VAL:HG22 | 2.47 | 0.44 |
| 8:E:32:VAL:HG23 | 8:E:33:VAL:N | 2.32 | 0.44 |
| 24:S:28:LYS:CD | 24:S:29:VAL:H | 2.31 | 0.44 |
| 26:F:98:PHE:C | 26:F:100:GLU:N | 2.71 | 0.44 |
| 2:B:564:C:H1' | 23:Q:36:GLN:OE1 | 2.17 | 0.44 |
| 2:B:2720:U:OP1 | 7:P:52:ARG:NH2 | 2.51 | 0.44 |
| 20:J:80:HIS:O | 20:J:81:ILE:C | 2.55 | 0.44 |
| 3:I:21:PRO:HB2 | 3:I:22:PRO:CD | 2.43 | 0.44 |
| 9:Y:47:ILE:HG21 | 9:Y:56:VAL:HG22 | 1.99 | 0.44 |
| 12:1:3:GLY:C | 12:1:5:ARG:N | 2.71 | 0.44 |
| 2:B:627:A:H4' | 2:B:628:G:H5' | 1.98 | 0.44 |
| 16:L:80:SER:HB3 | 16:L:115:GLU:OE2 | 2.18 | 0.44 |
| 19:H:97:ARG:HB3 | 19:H:112:LYS:HD3 | 1.98 | 0.44 |
| 27:G:88:LEU:HD13 | 27:G:93:TYR:HB3 | 1.99 | 0.44 |
| 19:H:126:GLY:O | 19:H:146:VAL:HG23 | 2.17 | 0.44 |
| 12:1:51:ALA:O | 12:1:52:LYS:C | 2.55 | 0.44 |
| 6:K:76:VAL:N | 7:P:72:VAL:HG23 | 2.26 | 0.44 |
| 17:M:35:ALA:CB | 17:M:100:LYS:H | 2.31 | 0.44 |
| 23:Q:24:TYR:CD1 | 23:Q:25:GLY:N | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:2041:U:H2' | 2:B:2042:A:C8 | 2.53 | 0.44 |
| 2:B:1047:G:H1' | 2:B:1110:G:H22 | 1.80 | 0.44 |
| 4:C:20:ASN:OD1 | 4:C:22:GLU:HG2 | 2.18 | 0.44 |
| 1:A:2:G:H3' | 1:A:2:G:OP2 | 2.17 | 0.44 |
| 4:C:157:ALA:C | 4:C:159:THR:H | 2.20 | 0.44 |
| 2:B:2109:U:H3 | 2:B:2180:U:H2' | 1.82 | 0.44 |
| 22:O:53:THR:O | 22:O:59:ALA:HB2 | 2.17 | 0.44 |
| 2:B:878:A:H1' | 2:B:899:A:H62 | 1.82 | 0.44 |
| 8:E:95:LYS:O | 8:E:96:VAL:HB | 2.17 | 0.44 |
| 2:B:263:G:H2' | 2:B:264:C:H6 | 1.82 | 0.44 |
| 22:O:110:ALA:HA | 22:O:113:ALA:HB3 | 1.98 | 0.44 |
| 2:B:52:A:C5 | 2:B:118:A:C2 | 3.05 | 0.44 |
| 3:I:5:GLN:HB2 | 3:I:30:GLN:OE1 | 2.18 | 0.44 |
| 2:B:41:C:H2' | 2:B:42:A:O4' | 2.16 | 0.44 |
| 2:B:1290:C:O2' | 2:B:1291:C:H5' | 2.17 | 0.44 |
| 2:B:1998:A:OP2 | 5:D:141:ARG:NH2 | 2.48 | 0.44 |
| 2:B:660:C:H2' | 2:B:661:A:C8 | 2.52 | 0.44 |
| 2:B:600:G:O4' | 8:E:100:MET:HE3 | 2.18 | 0.44 |
| 2:B:683:U:O5' | 2:B:683:U:H6 | 2.00 | 0.44 |
| 2:B:2018:G:H2' | 2:B:2019:A:H8 | 1.82 | 0.44 |
| 3:I:59:THR:O | 3:I:59:THR:HG23 | 2.18 | 0.44 |
| 5:D:56:LYS:HG3 | 5:D:58:ASN:HB2 | 1.99 | 0.44 |
| 2:B:1838:C:N4 | 2:B:1898:U:H2' | 2.32 | 0.44 |
| 17:M:34:LYS:HB3 | 17:M:129:THR:HG22 | 2.00 | 0.44 |
| 2:B:1099:G:O2' | 2:B:1100:C:H5' | 2.18 | 0.44 |
| 2:B:917:A:C2 | 2:B:918:A:H1' | 2.52 | 0.44 |
| 2:B:918:A:C2' | 2:B:919:U:H5' | 2.46 | 0.44 |
| 27:G:29:ASN:HD21 | 27:G:81:GLY:HA2 | 1.81 | 0.44 |
| 23:Q:91:ARG:HH12 | 28:R:10:LYS:CB | 2.23 | 0.44 |
| 17:M:38:ARG:HB3 | 17:M:98:PRO:HD3 | 1.99 | 0.44 |
| 29:T:45:ALA:HA | 29:T:48:GLN:CG | 2.47 | 0.44 |
| 29:T:29:THR:CG2 | 29:T:86:THR:HG22 | 2.47 | 0.44 |
| 21:N:70:THR:C | 21:N:72:ASP:H | 2.21 | 0.44 |
| 24:S:24:ILE:HG23 | 24:S:32:ALA:HB1 | 2.00 | 0.44 |
| 30:Z:6:GLN:NE2 | 30:Z:50:ARG:N | 2.65 | 0.44 |
| 2:B:1655:A:H2 | 2:B:2049:G:O3' | 2.01 | 0.44 |
| 5:D:113:SER:HB3 | 5:D:167:ASN:HA | 2.00 | 0.44 |
| 2:B:481:G:H1' | 2:B:506:G:N2 | 2.33 | 0.44 |
| 2:B:2556:C:H2' | 2:B:2557:G:O4' | 2.17 | 0.44 |
| 2:B:589:U:H2' | 2:B:590:A:H8 | 1.79 | 0.44 |
| 2:B:1921:G:H2' | 2:B:1922:G:H8 | 1.83 | 0.44 |
| 18:X:20:ASN:HD22 | 18:X:20:ASN:N | 2.14 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:2182:U:O2' | 2:B:2183:A:H5' | 2.17 | 0.44 |
| 2:B:657:U:H2' | 2:B:658:U:H6 | 1.82 | 0.44 |
| 2:B:572:A:OP2 | 28:R:80:ARG:NH2 | 2.50 | 0.44 |
| 2:B:2199:A:H3' | 2:B:2200:C:C6 | 2.52 | 0.44 |
| 26:F:15:LEU:HD13 | 26:F:28:PRO:HD2 | 1.99 | 0.44 |
| 2:B:1210:G:H5' | 2:B:1212:G:O4' | 2.17 | 0.44 |
| 2:B:2434:A:H2' | 2:B:2434:A:H8 | 1.68 | 0.44 |
| 8:E:7:ASP:N | 8:E:7:ASP:OD2 | 2.50 | 0.44 |
| 2:B:1310:G:C2' | 2:B:1311:G:H5' | 2.48 | 0.44 |
| 2:B:1064:C:H2' | 2:B:1065:U:O4' | 2.17 | 0.44 |
| 24:S:2:GLU:O | 24:S:3:THR:O | 2.36 | 0.44 |
| 2:B:925:A:O2' | 2:B:926:G:H5' | 2.18 | 0.44 |
| 16:L:105:ILE:HG22 | 16:L:106:GLU:N | 2.32 | 0.44 |
| 16:L:108:ALA:HB3 | 16:L:125:LEU:CD2 | 2.48 | 0.44 |
| 2:B:529:A:OP2 | 20:J:113:PRO:HD3 | 2.18 | 0.44 |
| 28:R:47:VAL:O | 28:R:49:ILE:N | 2.50 | 0.44 |
| 2:B:345:A:N3 | 2:B:346:A:N1 | 2.66 | 0.44 |
| 29:T:38:ALA:HB3 | 29:T:81:LYS:NZ | 2.33 | 0.44 |
| 26:F:34:THR:O | 26:F:89:THR:HA | 2.17 | 0.44 |
| 4:C:180:MET:HB2 | 4:C:268:ARG:CB | 2.44 | 0.44 |
| 2:B:2665:A:H2' | 2:B:2666:C:O2 | 2.18 | 0.44 |
| 2:B:2688:G:H1' | 2:B:2721:A:N6 | 2.32 | 0.44 |
| 2:B:2531:A:OP2 | 27:G:174:LYS:HB3 | 2.18 | 0.44 |
| 2:B:1548:A:H2' | 2:B:1549:A:H8 | 1.80 | 0.44 |
| 30:Z:63:GLY:O | 30:Z:67:VAL:HG23 | 2.18 | 0.44 |
| 6:K:20:MET:C | 6:K:41:ILE:HD12 | 2.38 | 0.44 |
| 6:K:43:ILE:CG2 | 6:K:46:ALA:HB2 | 2.45 | 0.44 |
| 29:T:2:ILE:O | 29:T:3:ARG:HD3 | 2.18 | 0.44 |
| 17:M:37:GLY:HA3 | 17:M:127:LYS:HZ3 | 1.81 | 0.44 |
| 29:T:73:ARG:CB | 29:T:73:ARG:HH21 | 2.26 | 0.44 |
| 2:B:2793:C:H2' | 2:B:2794:C:C6 | 2.52 | 0.44 |
| 4:C:29:PHE:CE2 | 4:C:31:PRO:HG2 | 2.53 | 0.44 |
| 2:B:1576:U:O2' | 2:B:1577:C:H5' | 2.18 | 0.44 |
| 2:B:1190:G:P | 16:L:32:GLY:HA2 | 2.57 | 0.44 |
| 2:B:540:C:O2' | 2:B:541:A:H5' | 2.18 | 0.44 |
| 2:B:40:U:H2' | 2:B:41:C:C6 | 2.52 | 0.44 |
| 2:B:863:A:O2' | 2:B:864:G:H5' | 2.17 | 0.44 |
| 10:O:35:GLU:OE1 | 10:O:44:ALA:HB3 | 2.18 | 0.44 |
| 31:W:31:LEU:O | 31:W:32:ALA:HB2 | 2.17 | 0.44 |
| 16:L:89:VAL:O | 16:L:89:VAL:HG13 | 2.18 | 0.44 |
| 20:J:36:LEU:HD11 | 20:J:122:LEU:HB2 | 1.98 | 0.44 |
| 23:Q:108:LEU:HA | 28:R:48:LYS:HD3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 28:R:4:VAL:O | 28:R:5:PHE:HB3 | 2.18 | 0.44 |
| 19:H:3:VAL:HG12 | 19:H:38:PRO:HA | 1.99 | 0.44 |
| 14:V:44:HIS:CE1 | 14:V:85:LYS:HB2 | 2.52 | 0.44 |
| 14:V:76:ASP:C | 17:M:136:MET:HE3 | 2.38 | 0.44 |
| 2:B:76:C:O2' | 2:B:77:G:H5' | 2.17 | 0.44 |
| 21:N:70:THR:OG1 | 21:N:75:ILE:HD11 | 2.17 | 0.44 |
| 24:S:24:ILE:CG2 | 24:S:32:ALA:HB1 | 2.48 | 0.44 |
| 26:F:1:ALA:HB1 | 26:F:4:HIS:HB3 | 2.00 | 0.44 |
| 2:B:2386:A:N3 | 31:W:38:ARG:HD2 | 2.33 | 0.44 |
| 20:J:81:ILE:HG23 | 20:J:82:GLY:N | 2.22 | 0.44 |
| 9:Y:2:LYS:CG | 9:Y:3:THR:H | 2.29 | 0.44 |
| 17:M:102:LEU:HB3 | 17:M:103:TYR:CD1 | 2.53 | 0.44 |
| 28:R:32:THR:HA | 28:R:61:ALA:O | 2.17 | 0.44 |
| 28:R:97:LYS:O | 28:R:98:ILE:HB | 2.18 | 0.44 |
| 8:E:170:ARG:HH22 | 8:E:176:ASP:HB3 | 1.83 | 0.44 |
| 2:B:20:C:O2' | 2:B:21:A:H5' | 2.17 | 0.44 |
| 2:B:21:A:O2' | 2:B:22:C:H5' | 2.18 | 0.44 |
| 20:J:73:VAL:HG23 | 20:J:74:TYR:H | 1.83 | 0.44 |
| 2:B:1883:U:H2' | 2:B:1884:G:C1' | 2.47 | 0.44 |
| 2:B:230:G:H2' | 2:B:231:A:H8 | 1.82 | 0.44 |
| 2:B:946:C:H2' | 2:B:947:A:C8 | 2.50 | 0.44 |
| 26:F:115:GLY:CA | 26:F:177:ARG:HB2 | 2.48 | 0.44 |
| 2:B:185:G:H2' | 2:B:186:G:H8 | 1.82 | 0.44 |
| 2:B:2341:G:H2' | 2:B:2342:C:H6 | 1.83 | 0.44 |
| 2:B:1422:G:H1' | 2:B:1495:A:H61 | 1.82 | 0.44 |
| 2:B:51:G:H1' | 2:B:118:A:N6 | 2.33 | 0.44 |
| 19:H:27:ARG:HG3 | 30:Z:60:ASP:OD1 | 2.18 | 0.44 |
| 5:D:4:LEU:HD23 | 5:D:101:PHE:CE1 | 2.52 | 0.44 |
| 29:T:5:GLU:HA | 29:T:8:LEU:HB2 | 1.99 | 0.44 |
| 22:O:109:ALA:HA | 22:O:112:GLU:OE2 | 2.18 | 0.44 |
| 13:3:37:THR:HA | 13:3:40:LYS:HE2 | 1.99 | 0.44 |
| 2:B:1830:C:H2' | 2:B:1831:G:H8 | 1.82 | 0.44 |
| 4:C:162:GLN:NE2 | 4:C:174:ARG:HE | 2.15 | 0.44 |
| 10:0:29:VAL:HA | 10:0:35:GLU:O | 2.17 | 0.44 |
| 2:B:1099:G:O5' | 3:I:3:LYS:C | 2.53 | 0.44 |
| 2:B:2353:G:N3 | 31:W:30:VAL:CG1 | 2.80 | 0.44 |
| 2:B:923:G:O2' | 2:B:924:G:H5' | 2.18 | 0.44 |
| 16:L:81:ASP:O | 16:L:82:LEU:HB2 | 2.18 | 0.44 |
| 18:X:31:GLN:CG | 18:X:37:LEU:HB2 | 2.42 | 0.44 |
| 23:Q:108:LEU:N | 28:R:48:LYS:HD3 | 2.32 | 0.44 |
| 5:D:187:LEU:O | 5:D:188:LEU:HD23 | 2.18 | 0.44 |
| 29:T:9:LYS:O | 29:T:10:VAL:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 17:M:72:PRO:O | 17:M:73:ILE:HB | 2.17 | 0.44 |
| 19:H:5:LEU:HD21 | 19:H:12:LEU:O | 2.17 | 0.44 |
| 7:P:27:VAL:HG21 | 7:P:73:PHE:CE2 | 2.53 | 0.44 |
| 2:B:1593:A:H2' | 2:B:1594:U:H6 | 1.82 | 0.44 |
| 20:J:74:TYR:CD1 | 20:J:92:MET:HG3 | 2.52 | 0.44 |
| 20:J:110:PRO:O | 20:J:115:GLY:HA3 | 2.18 | 0.44 |
| 2:B:2463:C:O2' | 2:B:2464:G:H5' | 2.18 | 0.44 |
| 2:B:814:C:H2' | 2:B:815:C:C6 | 2.53 | 0.44 |
| 5:D:171:THR:OG1 | 5:D:172:VAL:N | 2.48 | 0.44 |
| 2:B:2835:A:N6 | 2:B:2878:U:H2' | 2.32 | 0.44 |
| 2:B:693:A:H2' | 2:B:694:U:H6 | 1.82 | 0.44 |
| 3:I:90:GLY:C | 3:I:92:PRO:HD3 | 2.38 | 0.44 |
| 2:B:680:C:H2' | 2:B:681:G:C8 | 2.52 | 0.44 |
| 8:E:37:ALA:O | 8:E:39:ALA:N | 2.43 | 0.44 |
| 16:L:51:GLU:CD | 16:L:60:ARG:HH11 | 2.21 | 0.44 |
| 2:B:2368:C:H2' | 2:B:2369:A:H8 | 1.81 | 0.44 |
| 28:R:49:ILE:HD13 | 28:R:53:PHE:H | 1.83 | 0.44 |
| 27:G:85:LYS:HG2 | 27:G:85:LYS:O | 2.17 | 0.44 |
| 21:N:86:ARG:NE | 21:N:117:ASP:OD1 | 2.49 | 0.44 |
| 2:B:2846:G:OP1 | 7:P:52:ARG:NH1 | 2.50 | 0.44 |
| 8:E:62:GLN:HB2 | 8:E:62:GLN:HE21 | 1.56 | 0.44 |
| 2:B:2733:A:C8 | 2:B:2733:A:H3' | 2.53 | 0.44 |
| 4:C:76:VAL:O | 4:C:78:GLU:N | 2.51 | 0.44 |
| 25:U:11:ILE:CG2 | 25:U:70:ALA:HB3 | 2.48 | 0.44 |
| 2:B:2834:G:O6 | 2:B:2879:A:H2' | 2.17 | 0.44 |
| 22:O:30:ARG:HA | 22:O:35:ILE:HD13 | 1.99 | 0.44 |
| 2:B:2344:U:H4' | 2:B:2345:G:OP1 | 2.17 | 0.44 |
| 1:A:87:U:C2' | 1:A:88:C:O5' | 2.66 | 0.44 |
| 18:X:59:GLU:N | 18:X:59:GLU:OE2 | 2.50 | 0.44 |
| 2:B:6:A:H2' | 2:B:7:G:C8 | 2.53 | 0.44 |
| 2:B:338:G:N2 | 2:B:339:U:H1' | 2.32 | 0.44 |
| 4:C:4:LYS:HB3 | 4:C:5:CYS:H | 1.59 | 0.44 |
| 2:B:587:C:O2' | 16:L:19:LEU:HD13 | 2.18 | 0.44 |
| 2:B:782:A:N3 | 4:C:224:MET:HB3 | 2.33 | 0.44 |
| 2:B:2183:A:H2' | 2:B:2184:A:C8 | 2.52 | 0.44 |
| 2:B:738:G:O2' | 2:B:739:A:H5' | 2.18 | 0.44 |
| 2:B:2552:U:H2' | 2:B:2554:U:OP2 | 2.18 | 0.44 |
| 2:B:930:G:H1' | 9:Y:24:LEU:HD11 | 2.00 | 0.44 |
| 12:1:18:HIS:CD2 | 12:1:40:PRO:HD2 | 2.53 | 0.44 |
| 2:B:642:U:O2' | 2:B:644:A:N7 | 2.46 | 0.44 |
| 26:F:157:THR:C | 26:F:159:ALA:H | 2.20 | 0.44 |
| 7:P:84:SER:OG | 7:P:85:VAL:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 30:Z:17:ASN:HB2 | 30:Z:25:THR:HB | 2.00 | 0.44 |
| 2:B:2379:G:H4' | 22:O:21:LEU:CD1 | 2.32 | 0.44 |
| 5:D:13:ARG:HB2 | 5:D:21:SER:OG | 2.18 | 0.44 |
| 14:V:29:ILE:HG13 | 14:V:88:HIS:CE1 | 2.52 | 0.44 |
| 29:T:58:VAL:O | 29:T:58:VAL:HG13 | 2.17 | 0.44 |
| 7:P:9:GLN:HA | 7:P:12:MET:HB2 | 2.00 | 0.44 |
| 15:2:43:THR:O | 15:2:44:VAL:C | 2.56 | 0.44 |
| 2:B:2768:U:H2' | 2:B:2769:U:O4' | 2.18 | 0.44 |
| 27:G:93:TYR:C | 27:G:94:ARG:HG3 | 2.38 | 0.44 |
| 8:E:147:LEU:HB3 | 8:E:186:VAL:HG23 | 1.99 | 0.44 |
| 5:D:116:LYS:HG3 | 5:D:123:LYS:HE2 | 2.00 | 0.44 |
| 19:H:83:LYS:HZ2 | 19:H:83:LYS:HB3 | 1.82 | 0.44 |
| 27:G:101:VAL:O | 27:G:101:VAL:HG23 | 2.18 | 0.44 |
| 22:O:88:LYS:CE | 22:O:116:GLN:HB2 | 2.45 | 0.44 |
| 25:U:62:ALA:O | 25:U:63:ALA:HB3 | 2.18 | 0.44 |
| 5:D:14:ILE:HG12 | 5:D:14:ILE:O | 2.18 | 0.44 |
| 26:F:115:GLY:CA | 26:F:177:ARG:HD2 | 2.48 | 0.44 |
| 27:G:21:GLN:HB3 | 27:G:37:ASN:HB3 | 2.00 | 0.44 |
| 2:B:2215:C:O2' | 2:B:2216:G:H5' | 2.18 | 0.44 |
| 20:J:64:VAL:O | 20:J:65:THR:HG22 | 2.17 | 0.44 |
| 2:B:1957:C:H2' | 2:B:1958:C:H6 | 1.79 | 0.44 |
| 2:B:1799:G:N2 | 2:B:1818:U:O2' | 2.50 | 0.44 |
| 2:B:2197:U:O2' | 2:B:2198:A:H2' | 2.17 | 0.44 |
| 21:N:118:ARG:HE | 21:N:118:ARG:HB3 | 1.48 | 0.44 |
| 30:Z:20:HIS:O | 30:Z:21:ALA:HB3 | 2.18 | 0.44 |
| 23:Q:38:VAL:O | 23:Q:39:ILE:C | 2.57 | 0.44 |
| 27:G:155:PRO:HA | 27:G:170:THR:HG22 | 2.00 | 0.44 |
| 2:B:251:A:H2' | 2:B:252:G:O4' | 2.17 | 0.44 |
| 2:B:2759:G:H21 | 27:G:138:GLN:HG3 | 1.82 | 0.44 |
| 10:O:30:ASP:HB3 | 10:O:33:SER:O | 2.18 | 0.44 |
| 31:W:19:ARG:NE | 31:W:19:ARG:H | 2.16 | 0.43 |
| 28:R:3:ALA:HB2 | 28:R:101:ILE:HD11 | 2.00 | 0.43 |
| 17:M:69:PRO:C | 17:M:71:LYS:H | 2.21 | 0.43 |
| 26:F:92:GLY:O | 26:F:95:MET:HB3 | 2.18 | 0.43 |
| 20:J:18:VAL:HG22 | 20:J:19:ASP:N | 2.33 | 0.43 |
| 2:B:2072:C:C2' | 2:B:2073:C:H5' | 2.48 | 0.43 |
| 16:L:116:VAL:HG22 | 16:L:117:THR:N | 2.33 | 0.43 |
| 2:B:851:C:O2' | 9:Y:42:ALA:HA | 2.17 | 0.43 |
| 2:B:927:A:H2' | 2:B:928:A:C8 | 2.53 | 0.43 |
| 25:U:18:LYS:HB3 | 25:U:19:GLY:H | 1.61 | 0.43 |
| 25:U:53:GLN:HG2 | 25:U:53:GLN:O | 2.18 | 0.43 |
| 27:G:152:ARG:HD2 | 27:G:152:ARG:HA | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 12:1:24:LYS:HE3 | 12:1:29:LYS:O | 2.18 | 0.43 |
| 13:3:21:PHE:HE1 | 13:3:58:ILE:HG12 | 1.83 | 0.43 |
| 2:B:1829:A:HO2' | 4:C:14:HIS:CD2 | 2.35 | 0.43 |
| 2:B:154:U:H2' | 2:B:155:A:H8 | 1.83 | 0.43 |
| 21:N:20:MET:HG3 | 21:N:21:PHE:N | 2.33 | 0.43 |
| 2:B:1495:A:H2' | 2:B:1496:A:C8 | 2.53 | 0.43 |
| 2:B:1450:G:C6 | 2:B:1451:C:N4 | 2.86 | 0.43 |
| 2:B:1451:C:H4' | 2:B:1452:G:H5' | 2.00 | 0.43 |
| 2:B:765:C:O2' | 2:B:766:U:H5' | 2.18 | 0.43 |
| 2:B:1258:U:H2' | 2:B:1259:G:C8 | 2.53 | 0.43 |
| 2:B:2376:A:H2' | 2:B:2377:A:O4' | 2.18 | 0.43 |
| 2:B:1221:C:O2' | 2:B:1222:U:H5' | 2.17 | 0.43 |
| 2:B:2868:A:H2' | 2:B:2869:G:H8 | 1.83 | 0.43 |
| 2:B:1560:G:H2' | 2:B:1561:C:C6 | 2.52 | 0.43 |
| 28:R:86:GLN:HB2 | 28:R:86:GLN:HE21 | 1.53 | 0.43 |
| 22:O:111:ARG:HB2 | 22:O:117:PHE:CZ | 2.53 | 0.43 |
| 2:B:1239:G:H5'' | 35:B:4039:HOH:O | 2.16 | 0.43 |
| 18:X:58:ASN:O | 18:X:61:ALA:N | 2.51 | 0.43 |
| 1:A:46:A:H2' | 1:A:47:C:O4' | 2.18 | 0.43 |
| 2:B:2577:A:H5'' | 2:B:2578:G:H5' | 2.00 | 0.43 |
| 24:S:10:ALA:HB3 | 24:S:101:SER:HB2 | 1.99 | 0.43 |
| 20:J:12:LYS:O | 20:J:13:ARG:HB2 | 2.18 | 0.43 |
| 23:Q:4:LYS:HE3 | 23:Q:4:LYS:HB3 | 1.76 | 0.43 |
| 26:F:111:ARG:O | 26:F:112:ASP:HB2 | 2.18 | 0.43 |
| 26:F:31:GLU:O | 26:F:32:LYS:O | 2.37 | 0.43 |
| 10:O:39:ARG:O | 10:O:40:HIS:HB2 | 2.18 | 0.43 |
| 30:Z:10:LYS:O | 30:Z:31:PRO:HG2 | 2.18 | 0.43 |
| 16:L:29:LYS:C | 16:L:30:THR:HG23 | 2.37 | 0.43 |
| 2:B:2544:G:H1' | 2:B:2646:C:H5' | 2.00 | 0.43 |
| 16:L:79:LEU:H | 16:L:113:ALA:HB2 | 1.84 | 0.43 |
| 27:G:88:LEU:HD11 | 27:G:94:ARG:CA | 2.48 | 0.43 |
| 25:U:81:ARG:HB2 | 25:U:96:LYS:CG | 2.47 | 0.43 |
| 2:B:2821:A:OP1 | 5:D:114:LYS:O | 2.36 | 0.43 |
| 10:O:38:LEU:HD13 | 10:O:41:HIS:NE2 | 2.33 | 0.43 |
| 14:V:40:ILE:N | 14:V:40:ILE:HD13 | 2.30 | 0.43 |
| 26:F:40:GLY:O | 26:F:41:GLU:C | 2.56 | 0.43 |
| 6:K:98:ARG:N | 6:K:98:ARG:HE | 2.16 | 0.43 |
| 2:B:2794:C:H2' | 2:B:2795:C:C6 | 2.53 | 0.43 |
| 22:O:71:ALA:CB | 22:O:102:ARG:HB3 | 2.48 | 0.43 |
| 6:K:12:ASP:OD2 | 6:K:85:VAL:HG13 | 2.18 | 0.43 |
| 2:B:877:A:H2' | 2:B:900:A:H61 | 1.83 | 0.43 |
| 2:B:2439:A:H4' | 2:B:2440:C:O5' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 18:X:22:LEU:HD12 | 18:X:23:ARG:HG2 | 2.00 | 0.43 |
| 2:B:1126:A:OP1 | 2:B:1126:A:C8 | 2.71 | 0.43 |
| 2:B:1312:U:O4 | 29:T:64:LYS:HG2 | 2.18 | 0.43 |
| 2:B:2389:G:H5' | 2:B:2390:U:O4' | 2.18 | 0.43 |
| 2:B:692:C:H2' | 2:B:693:A:H8 | 1.82 | 0.43 |
| 2:B:599:A:N3 | 8:E:100:MET:HE1 | 2.33 | 0.43 |
| 2:B:2047:C:H2' | 2:B:2048:G:C8 | 2.53 | 0.43 |
| 2:B:1478:G:O2' | 2:B:1479:G:H5' | 2.18 | 0.43 |
| 2:B:1766:G:O2' | 2:B:1767:G:H5' | 2.17 | 0.43 |
| 2:B:679:C:H2' | 2:B:680:C:H6 | 1.83 | 0.43 |
| 2:B:2758:A:C2' | 2:B:2759:G:H5' | 2.48 | 0.43 |
| 20:J:7:LYS:C | 20:J:9:GLU:H | 2.22 | 0.43 |
| 5:D:49:GLN:HE22 | 5:D:67:HIS:CE1 | 2.35 | 0.43 |
| 2:B:1156:A:P | 23:Q:54:ARG:HH21 | 2.41 | 0.43 |
| 20:J:44:TYR:CD2 | 23:Q:59:LEU:HD11 | 2.53 | 0.43 |
| 20:J:44:TYR:CZ | 23:Q:59:LEU:HD11 | 2.53 | 0.43 |
| 7:P:64:SER:O | 7:P:66:GLY:N | 2.51 | 0.43 |
| 29:T:53:VAL:HG12 | 29:T:54:GLU:H | 1.82 | 0.43 |
| 3:I:72:THR:OG1 | 3:I:73:PRO:HD2 | 2.18 | 0.43 |
| 26:F:33:ILE:HD12 | 26:F:95:MET:HG2 | 1.99 | 0.43 |
| 2:B:1082:U:C2 | 2:B:1086:A:N1 | 2.86 | 0.43 |
| 4:C:94:LEU:HA | 4:C:100:ARG:HA | 2.00 | 0.43 |
| 26:F:57:ALA:HB2 | 26:F:64:PRO:CD | 2.48 | 0.43 |
| 2:B:2415:G:H2' | 2:B:2416:C:C6 | 2.53 | 0.43 |
| 8:E:109:LEU:O | 8:E:112:LEU:HB2 | 2.17 | 0.43 |
| 11:4:11:CYS:HB3 | 11:4:33:HIS:CE1 | 2.53 | 0.43 |
| 4:C:250:GLN:HG2 | 4:C:254:LYS:HG2 | 1.99 | 0.43 |
| 25:U:41:VAL:C | 25:U:42:LYS:HD2 | 2.38 | 0.43 |
| 2:B:633:A:H2' | 2:B:634:C:O4' | 2.18 | 0.43 |
| 2:B:833:A:H1' | 16:L:52:GLY:N | 2.33 | 0.43 |
| 2:B:2692:G:O2' | 2:B:2693:G:H5' | 2.18 | 0.43 |
| 26:F:66:ILE:HA | 26:F:85:GLY:O | 2.17 | 0.43 |
| 2:B:2636:C:H2' | 2:B:2637:U:H6 | 1.82 | 0.43 |
| 2:B:957:C:N4 | 2:B:2459:A:C8 | 2.87 | 0.43 |
| 1:A:54:G:O2' | 1:A:55:U:H5' | 2.18 | 0.43 |
| 26:F:59:ILE:H | 26:F:59:ILE:HG13 | 1.39 | 0.43 |
| 1:A:20:G:H2' | 1:A:21:G:H8 | 1.82 | 0.43 |
| 2:B:2651:C:O2' | 2:B:2652:C:H5' | 2.18 | 0.43 |
| 2:B:368:A:O2' | 2:B:369:U:H5' | 2.18 | 0.43 |
| 16:L:125:LEU:N | 16:L:143:GLU:HG3 | 2.31 | 0.43 |
| 4:C:142:ASN:CG | 4:C:142:ASN:O | 2.55 | 0.43 |
| 23:Q:104:ALA:HA | 28:R:46:GLU:CD | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 23:Q:63:ARG:NH2 | 23:Q:95:ALA:O | 2.51 | 0.43 |
| 23:Q:93:ILE:HG23 | 23:Q:94:LEU:N | 2.33 | 0.43 |
| 24:S:60:HIS:ND1 | 24:S:61:ASN:N | 2.66 | 0.43 |
| 2:B:2032:G:H21 | 5:D:151:THR:N | 2.15 | 0.43 |
| 5:D:151:THR:N | 5:D:152:PRO:CD | 2.81 | 0.43 |
| 30:Z:59:ILE:CD1 | 30:Z:67:VAL:HG21 | 2.49 | 0.43 |
| 1:A:7:G:O2' | 1:A:8:C:H5' | 2.19 | 0.43 |
| 2:B:850:U:O2' | 9:Y:22:THR:HA | 2.18 | 0.43 |
| 9:Y:8:GLN:HG2 | 9:Y:31:ILE:HA | 2.00 | 0.43 |
| 7:P:91:VAL:HG11 | 7:P:96:LEU:HD21 | 1.99 | 0.43 |
| 16:L:103:ILE:H | 16:L:103:ILE:CD1 | 2.27 | 0.43 |
| 1:A:3:C:H2' | 1:A:4:C:O4' | 2.17 | 0.43 |
| 2:B:419:U:H2' | 2:B:420:C:H6 | 1.80 | 0.43 |
| 2:B:1789:A:H2' | 2:B:1790:C:O4' | 2.18 | 0.43 |
| 2:B:948:C:H2' | 2:B:949:G:C8 | 2.53 | 0.43 |
| 2:B:934:U:H2' | 2:B:935:C:H6 | 1.80 | 0.43 |
| 2:B:958:U:N3 | 17:M:16:ARG:HB3 | 2.33 | 0.43 |
| 19:H:129:GLU:HB3 | 19:H:143:ILE:HG12 | 1.99 | 0.43 |
| 17:M:63:ILE:N | 17:M:63:ILE:HD12 | 2.34 | 0.43 |
| 2:B:2315:G:H2' | 2:B:2316:G:C8 | 2.53 | 0.43 |
| 2:B:679:C:H2' | 2:B:680:C:C6 | 2.54 | 0.43 |
| 2:B:2630:G:O2' | 2:B:2631:G:H5' | 2.18 | 0.43 |
| 2:B:2367:G:O2' | 2:B:2368:C:H5' | 2.18 | 0.43 |
| 31:W:32:ALA:C | 31:W:34:SER:H | 2.21 | 0.43 |
| 25:U:84:PHE:HD2 | 25:U:91:LYS:HG2 | 1.84 | 0.43 |
| 23:Q:86:SER:O | 28:R:52:PRO:HD3 | 2.19 | 0.43 |
| 29:T:40:LYS:O | 29:T:43:ILE:HB | 2.19 | 0.43 |
| 3:I:54:ILE:HD11 | 3:I:71:LYS:N | 2.33 | 0.43 |
| 24:S:24:ILE:CG2 | 24:S:71:VAL:HG11 | 2.36 | 0.43 |
| 2:B:282:A:C2' | 2:B:283:G:H5' | 2.48 | 0.43 |
| 26:F:175:PRO:O | 26:F:176:PHE:HB2 | 2.17 | 0.43 |
| 5:D:90:PHE:O | 5:D:91:THR:C | 2.57 | 0.43 |
| 1:A:8:C:OP1 | 22:O:15:ARG:NH2 | 2.51 | 0.43 |
| 16:L:116:VAL:HG13 | 16:L:117:THR:N | 2.22 | 0.43 |
| 21:N:90:ARG:HB3 | 21:N:94:TYR:HE1 | 1.83 | 0.43 |
| 6:K:70:ARG:HB3 | 6:K:76:VAL:CG2 | 2.44 | 0.43 |
| 8:E:176:ASP:O | 8:E:180:LEU:HG | 2.18 | 0.43 |
| 20:J:96:ARG:NE | 20:J:99:ARG:HD2 | 2.32 | 0.43 |
| 2:B:722:A:H2' | 2:B:723:C:C6 | 2.54 | 0.43 |
| 2:B:2137:U:O2' | 2:B:2138:G:H5' | 2.18 | 0.43 |
| 14:V:65:VAL:O | 14:V:68:LYS:HG2 | 2.17 | 0.43 |
| 22:O:35:ILE:HG13 | 22:O:71:ALA:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:458:G:H22 | 2:B:469:G:H2' | 1.83 | 0.43 |
| 2:B:904:G:H2' | 2:B:905:A:C8 | 2.54 | 0.43 |
| 2:B:1401:G:H2' | 2:B:1402:U:C6 | 2.53 | 0.43 |
| 8:E:153:LEU:HG | 8:E:154:ASP:N | 2.34 | 0.43 |
| 21:N:71:ARG:HH21 | 21:N:71:ARG:CG | 2.31 | 0.43 |
| 2:B:2322:A:N6 | 2:B:2333:A:H62 | 2.16 | 0.43 |
| 2:B:1027:A:N3 | 2:B:2488:G:H5'' | 2.34 | 0.43 |
| 2:B:863:A:H2' | 2:B:864:G:H8 | 1.84 | 0.43 |
| 2:B:527:C:O2 | 2:B:527:C:O4' | 2.37 | 0.43 |
| 2:B:83:A:H2' | 2:B:84:A:C8 | 2.53 | 0.43 |
| 2:B:15:G:O2' | 2:B:16:C:H5' | 2.18 | 0.43 |
| 31:W:59:PHE:O | 31:W:60:ALA:CB | 2.67 | 0.43 |
| 16:L:85:VAL:HG22 | 16:L:94:THR:HG21 | 2.01 | 0.43 |
| 5:D:175:LEU:HD21 | 5:D:191:GLY:O | 2.19 | 0.43 |
| 5:D:13:ARG:HD2 | 7:P:55:HIS:ND1 | 2.34 | 0.43 |
| 4:C:171:VAL:HG23 | 4:C:185:ALA:CB | 2.48 | 0.43 |
| 4:C:89:ASN:HD22 | 4:C:89:ASN:HA | 1.54 | 0.43 |
| 27:G:84:LYS:HG3 | 27:G:132:LEU:N | 2.33 | 0.43 |
| 24:S:73:LYS:HE3 | 24:S:74:ILE:N | 2.21 | 0.43 |
| 10:O:39:ARG:HH11 | 10:O:39:ARG:HG3 | 1.83 | 0.43 |
| 20:J:58:ASN:O | 20:J:60:ASP:N | 2.44 | 0.43 |
| 19:H:10:ALA:C | 19:H:12:LEU:H | 2.22 | 0.43 |
| 9:Y:12:ALA:HB2 | 9:Y:53:MET:CE | 2.48 | 0.43 |
| 2:B:141:G:C3' | 2:B:141:G:N3 | 2.78 | 0.43 |
| 9:Y:8:GLN:CG | 9:Y:31:ILE:HA | 2.49 | 0.43 |
| 9:Y:7:THR:HA | 9:Y:34:THR:HA | 2.00 | 0.43 |
| 8:E:117:ARG:HA | 8:E:185:LYS:HZ2 | 1.82 | 0.43 |
| 8:E:148:ILE:HD13 | 8:E:187:VAL:CG2 | 2.48 | 0.43 |
| 26:F:53:ALA:O | 26:F:64:PRO:HG2 | 2.19 | 0.43 |
| 26:F:40:GLY:N | 26:F:84:ILE:O | 2.50 | 0.43 |
| 13:3:22:LYS:HA | 13:3:47:ALA:O | 2.19 | 0.43 |
| 2:B:1881:C:H2' | 2:B:1882:U:O4' | 2.19 | 0.43 |
| 25:U:40:LEU:HD12 | 25:U:40:LEU:H | 1.84 | 0.43 |
| 2:B:1353:A:H2' | 2:B:1354:A:H8 | 1.82 | 0.43 |
| 16:L:56:PRO:HD2 | 16:L:59:ARG:HG3 | 2.01 | 0.43 |
| 2:B:304:U:O2' | 2:B:305:C:H5' | 2.18 | 0.43 |
| 2:B:659:G:N2 | 8:E:30:GLN:NE2 | 2.65 | 0.43 |
| 2:B:1465:G:H2' | 2:B:1466:U:C6 | 2.54 | 0.43 |
| 1:A:115:A:O2' | 1:A:116:G:H5' | 2.18 | 0.43 |
| 2:B:323:C:H2' | 8:E:163:ASN:OD1 | 2.19 | 0.43 |
| 6:K:66:LYS:HZ1 | 6:K:81:GLY:HA2 | 1.84 | 0.43 |
| 2:B:622:G:O2' | 2:B:623:C:H5' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:B:1933:G:O2' | 2:B:1974:C:H4' | 2.18 | 0.43 |
| 2:B:661:A:H1' | 16:L:12:SER:O | 2.18 | 0.43 |
| 2:B:68:G:H2' | 2:B:69:C:C6 | 2.53 | 0.43 |
| 2:B:1607:C:H4' | 2:B:1608:A:O5' | 2.19 | 0.43 |
| 2:B:1063:G:O2' | 2:B:1064:C:H5' | 2.18 | 0.43 |
| 2:B:1851:U:O2' | 2:B:1852:U:H5' | 2.19 | 0.43 |
| 2:B:213:A:O2' | 2:B:214:G:H5' | 2.19 | 0.43 |
| 2:B:1664:A:H1' | 2:B:2726:A:C2 | 2.53 | 0.43 |
| 13:3:56:LEU:O | 13:3:59:ALA:HB3 | 2.19 | 0.43 |
| 1:A:35:C:H2' | 1:A:36:C:H5' | 2.01 | 0.43 |
| 2:B:2015:A:C2 | 10:0:2:VAL:HG22 | 2.53 | 0.43 |
| 2:B:24:G:H1' | 24:S:77:ASP:HB3 | 1.99 | 0.43 |
| 31:W:19:ARG:HA | 31:W:34:SER:HA | 2.00 | 0.43 |
| 31:W:43:LYS:CD | 31:W:79:ILE:HD11 | 2.45 | 0.43 |
| 27:G:24:THR:HB | 27:G:34:ARG:CD | 2.48 | 0.43 |
| 23:Q:51:GLN:O | 23:Q:54:ARG:HB2 | 2.18 | 0.43 |
| 19:H:41:LYS:HA | 19:H:44:ILE:CD1 | 2.49 | 0.43 |
| 2:B:78:U:O2' | 2:B:79:C:H5' | 2.19 | 0.43 |
| 29:T:38:ALA:HB3 | 29:T:81:LYS:HD3 | 2.00 | 0.43 |
| 2:B:1182:G:H2' | 2:B:1183:U:O4' | 2.18 | 0.43 |
| 6:K:47:ILE:HG23 | 6:K:48:PRO:CD | 2.49 | 0.43 |
| 9:Y:43:ILE:O | 9:Y:47:ILE:HG12 | 2.18 | 0.43 |
| 4:C:76:VAL:HA | 4:C:113:ASP:O | 2.18 | 0.43 |
| 17:M:26:VAL:HB | 17:M:104:GLU:OE2 | 2.18 | 0.43 |
| 2:B:181:A:H1' | 2:B:435:C:H5' | 2.01 | 0.43 |
| 21:N:34:ILE:HB | 21:N:113:ILE:CG2 | 2.47 | 0.43 |
| 28:R:21:ARG:HB3 | 28:R:95:ASP:OD1 | 2.19 | 0.43 |
| 1:A:28:C:H2' | 1:A:29:A:O4' | 2.18 | 0.43 |
| 2:B:1795:C:O2' | 2:B:1796:U:H5' | 2.19 | 0.43 |
| 20:J:30:THR:CG2 | 20:J:31:GLU:N | 2.81 | 0.43 |
| 1:A:93:C:O2' | 1:A:94:A:H5' | 2.18 | 0.43 |
| 2:B:1241:A:N3 | 2:B:1241:A:O4' | 2.51 | 0.43 |
| 5:D:101:PHE:O | 5:D:102:ALA:HB2 | 2.18 | 0.43 |
| 2:B:2458:G:N3 | 2:B:2458:G:H2' | 2.33 | 0.43 |
| 4:C:211:ARG:HD2 | 4:C:211:ARG:HA | 1.86 | 0.43 |
| 6:K:121:GLU:O | 6:K:122:VAL:C | 2.56 | 0.43 |
| 1:A:65:U:C2' | 1:A:66:A:H5' | 2.49 | 0.43 |
| 27:G:54:ARG:HD3 | 27:G:54:ARG:C | 2.39 | 0.43 |
| 2:B:2520:C:O2' | 2:B:2521:C:H5' | 2.19 | 0.43 |
| 2:B:1145:C:O2' | 2:B:1146:C:H5' | 2.19 | 0.43 |
| 2:B:2519:U:C6 | 2:B:2542:A:N6 | 2.87 | 0.43 |
| 2:B:1700:A:H2' | 2:B:1701:A:H5' | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:U:43:LYS:C | 25:U:43:LYS:HD3 | 2.38 | 0.43 |
| 2:B:920:A:H2' | 2:B:921:C:C6 | 2.53 | 0.43 |
| 2:B:922:C:H2' | 2:B:923:G:C8 | 2.54 | 0.43 |
| 27:G:22:VAL:HG13 | 27:G:36:LEU:HD13 | 1.99 | 0.43 |
| 19:H:89:LYS:HD2 | 19:H:89:LYS:N | 2.33 | 0.43 |
| 3:I:52:LEU:HD13 | 3:I:81:LYS:NZ | 2.33 | 0.43 |
| 27:G:102:ILE:HG13 | 27:G:116:LEU:CD1 | 2.49 | 0.43 |
| 24:S:33:LEU:CD2 | 24:S:48:LYS:HE3 | 2.49 | 0.43 |
| 17:M:42:THR:HA | 17:M:93:VAL:HA | 2.00 | 0.43 |
| 26:F:172:PHE:C | 26:F:174:PHE:H | 2.22 | 0.43 |
| 2:B:372:G:N7 | 30:Z:57:ARG:HB3 | 2.33 | 0.43 |
| 2:B:138:U:H2' | 2:B:140:C:C1' | 2.49 | 0.43 |
| 2:B:626:A:H2' | 16:L:78:ARG:NH1 | 2.33 | 0.43 |
| 19:H:110:VAL:HG23 | 19:H:132:PHE:CD2 | 2.54 | 0.43 |
| 4:C:93:VAL:HG13 | 4:C:94:LEU:N | 2.34 | 0.43 |
| 12:1:29:LYS:HA | 12:1:31:GLU:OE1 | 2.18 | 0.43 |
| 9:Y:35:VAL:HG22 | 9:Y:36:GLU:N | 2.33 | 0.43 |
| 2:B:1871:A:H2' | 2:B:1872:A:C8 | 2.54 | 0.43 |
| 2:B:1655:A:C2 | 2:B:2049:G:H4' | 2.54 | 0.43 |
| 21:N:28:LEU:HD23 | 21:N:113:ILE:HG23 | 2.01 | 0.43 |
| 10:0:42:ILE:HG12 | 21:N:99:LYS:O | 2.18 | 0.43 |
| 22:O:31:THR:HG23 | 22:O:34:HIS:O | 2.19 | 0.43 |
| 28:R:78:ARG:NH2 | 28:R:78:ARG:HG3 | 2.33 | 0.43 |
| 2:B:1334:G:O2' | 2:B:1335:C:H5' | 2.19 | 0.43 |
| 21:N:96:ARG:HG2 | 21:N:96:ARG:NH2 | 2.34 | 0.43 |
| 2:B:1718:G:H2' | 2:B:1719:G:H8 | 1.82 | 0.43 |
| 22:O:56:LYS:HG2 | 22:O:60:GLU:CD | 2.39 | 0.43 |
| 2:B:116:C:H1' | 2:B:127:A:N3 | 2.33 | 0.43 |
| 2:B:1729:U:C5' | 2:B:1730:C:H4' | 2.48 | 0.43 |
| 20:J:64:VAL:CG1 | 20:J:68:LYS:HB2 | 2.48 | 0.43 |
| 19:H:27:ARG:NH1 | 30:Z:60:ASP:HA | 2.34 | 0.43 |
| 2:B:775:G:H4' | 2:B:776:G:H5' | 2.00 | 0.43 |
| 6:K:88:ASN:ND2 | 6:K:89:ASN:N | 2.67 | 0.43 |
| 2:B:2863:C:H2' | 2:B:2864:G:H8 | 1.84 | 0.43 |
| 4:C:120:ASP:OD2 | 4:C:120:ASP:N | 2.51 | 0.43 |
| 23:Q:35:PHE:C | 23:Q:37:ALA:H | 2.22 | 0.43 |
| 2:B:2828:G:O2' | 2:B:2829:A:H5' | 2.19 | 0.43 |
| 2:B:291:G:O2' | 2:B:292:U:H5' | 2.18 | 0.43 |
| 4:C:128:THR:HG22 | 4:C:129:LEU:N | 2.34 | 0.43 |
| 25:U:86:PHE:CZ | 25:U:87:GLU:HG3 | 2.54 | 0.43 |
| 27:G:28:LYS:O | 27:G:30:GLY:N | 2.52 | 0.43 |
| 23:Q:83:LYS:NZ | 23:Q:83:LYS:HA | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 23:Q:89:ILE:O | 23:Q:90:ASP:HB2 | 2.19 | 0.43 |
| 4:C:45:ASN:ND2 | 4:C:45:ASN:H | 2.17 | 0.43 |
| 2:B:704:G:O2' | 2:B:727:A:N6 | 2.52 | 0.43 |
| 29:T:22:THR:O | 29:T:25:GLU:HB3 | 2.18 | 0.43 |
| 21:N:62:ASN:O | 21:N:66:ALA:HB2 | 2.19 | 0.43 |
| 17:M:123:LYS:O | 17:M:124:LEU:C | 2.57 | 0.43 |
| 2:B:784:G:N1 | 4:C:227:VAL:HG11 | 2.34 | 0.43 |
| 9:Y:23:LEU:CD1 | 9:Y:28:LEU:HB2 | 2.47 | 0.43 |
| 5:D:62:LYS:N | 5:D:63:PRO:CD | 2.82 | 0.43 |
| 2:B:2798:U:H4' | 2:B:2800:A:C2 | 2.53 | 0.43 |
| 20:J:72:LYS:CG | 20:J:89:PHE:HB2 | 2.49 | 0.43 |
| 2:B:1841:U:H2' | 2:B:1842:G:H8 | 1.82 | 0.43 |
| 2:B:459:U:C2' | 2:B:460:A:H5' | 2.49 | 0.43 |
| 2:B:266:G:H3' | 2:B:267:C:H5'' | 2.01 | 0.43 |
| 2:B:2536:G:H2' | 2:B:2537:U:C6 | 2.53 | 0.43 |
| 2:B:987:C:H2' | 2:B:988:A:O4' | 2.19 | 0.43 |
| 2:B:1339:G:N2 | 2:B:1603:A:H1' | 2.34 | 0.43 |
| 2:B:1210:G:H5'' | 2:B:1211:C:H3' | 1.99 | 0.43 |
| 2:B:81:G:H2' | 2:B:82:U:O4' | 2.18 | 0.43 |
| 2:B:1098:A:O5' | 3:I:3:LYS:CG | 2.66 | 0.43 |
| 16:L:77:ILE:CD1 | 16:L:95:LEU:HD22 | 2.49 | 0.43 |
| 4:C:140:VAL:CG2 | 4:C:163:ILE:HG12 | 2.49 | 0.43 |
| 18:X:39:GLN:HG3 | 18:X:42:LEU:HD22 | 2.01 | 0.43 |
| 27:G:25:ILE:HD11 | 27:G:71:LEU:HD11 | 2.01 | 0.43 |
| 20:J:25:LEU:HD13 | 20:J:25:LEU:C | 2.39 | 0.43 |
| 20:J:26:GLY:HA2 | 20:J:29:ALA:HB3 | 2.01 | 0.43 |
| 20:J:28:LEU:HD23 | 20:J:29:ALA:N | 2.34 | 0.43 |
| 4:C:43:ASN:HB3 | 4:C:45:ASN:ND2 | 2.32 | 0.43 |
| 19:H:118:PRO:O | 19:H:119:ASN:HB3 | 2.19 | 0.43 |
| 14:V:31:TYR:O | 14:V:92:VAL:HG13 | 2.19 | 0.43 |
| 29:T:28:ASN:ND2 | 29:T:29:THR:HG23 | 2.34 | 0.43 |
| 26:F:71:LYS:HG2 | 26:F:71:LYS:O | 2.18 | 0.43 |
| 3:I:128:ILE:HA | 3:I:131:THR:HG23 | 2.00 | 0.43 |
| 27:G:121:THR:O | 27:G:132:LEU:HA | 2.19 | 0.43 |
| 27:G:83:THR:C | 27:G:84:LYS:HD3 | 2.40 | 0.43 |
| 17:M:69:PRO:HA | 17:M:94:ALA:HB2 | 2.01 | 0.43 |
| 15:2:13:ASN:O | 15:2:17:GLY:HA3 | 2.18 | 0.43 |
| 22:O:26:LEU:HD13 | 22:O:39:VAL:HG23 | 2.00 | 0.43 |
| 3:I:45:THR:O | 3:I:48:ILE:HG22 | 2.18 | 0.43 |
| 8:E:48:THR:N | 8:E:51:GLU:HG3 | 2.34 | 0.43 |
| 23:Q:27:ARG:HG3 | 23:Q:27:ARG:NH1 | 2.34 | 0.43 |
| 26:F:49:LEU:HD13 | 26:F:50:ASP:N | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:2109:U:H2' | 2:B:2180:U:N3 | 2.31 | 0.43 |
| 2:B:878:A:H1' | 2:B:899:A:N7 | 2.34 | 0.43 |
| 27:G:106:LEU:O | 27:G:108:PHE:N | 2.52 | 0.43 |
| 6:K:107:LEU:H | 6:K:107:LEU:HD12 | 1.84 | 0.43 |
| 2:B:2604:U:O2' | 2:B:2605:U:H5' | 2.19 | 0.43 |
| 2:B:2514:U:H2' | 2:B:2515:C:H6 | 1.83 | 0.43 |
| 2:B:1210:G:P | 2:B:1212:G:H5' | 2.59 | 0.43 |
| 2:B:907:G:O2' | 2:B:908:C:H5' | 2.19 | 0.43 |
| 2:B:1987:A:H2' | 2:B:1988:G:H8 | 1.84 | 0.43 |
| 12:1:39:ASP:OD1 | 12:1:41:VAL:HB | 2.19 | 0.43 |
| 2:B:922:C:HO2' | 31:W:25:PHE:HZ | 1.64 | 0.42 |
| 4:C:117:SER:HB2 | 4:C:128:THR:HB | 2.01 | 0.42 |
| 5:D:13:ARG:HG3 | 5:D:15:PHE:CE1 | 2.54 | 0.42 |
| 14:V:29:ILE:HD13 | 14:V:31:TYR:CE2 | 2.54 | 0.42 |
| 4:C:131:MET:HE2 | 4:C:187:CYS:O | 2.19 | 0.42 |
| 29:T:39:THR:HG23 | 29:T:42:GLU:H | 1.83 | 0.42 |
| 29:T:47:VAL:HB | 29:T:55:VAL:HG21 | 2.00 | 0.42 |
| 4:C:80:LEU:HD22 | 4:C:109:LEU:HD12 | 2.01 | 0.42 |
| 3:I:54:ILE:HG23 | 3:I:54:ILE:O | 2.19 | 0.42 |
| 2:B:1455:G:H5' | 21:N:60:VAL:HG21 | 2.01 | 0.42 |
| 2:B:2654:A:N6 | 2:B:2666:C:OP2 | 2.50 | 0.42 |
| 9:Y:7:THR:HG23 | 9:Y:34:THR:OG1 | 2.18 | 0.42 |
| 16:L:78:ARG:HB3 | 16:L:113:ALA:HB2 | 2.00 | 0.42 |
| 27:G:94:ARG:HA | 27:G:128:THR:HG22 | 2.01 | 0.42 |
| 17:M:126:ILE:HG22 | 17:M:127:LYS:N | 2.34 | 0.42 |
| 8:E:138:LEU:HB3 | 8:E:143:LEU:O | 2.19 | 0.42 |
| 8:E:160:ALA:O | 8:E:161:ALA:HB3 | 2.19 | 0.42 |
| 11:4:10:LEU:HD12 | 11:4:33:HIS:CA | 2.46 | 0.42 |
| 4:C:156:SER:HB3 | 4:C:159:THR:CG2 | 2.49 | 0.42 |
| 17:M:31:PHE:HB3 | 17:M:130:PHE:CZ | 2.54 | 0.42 |
| 22:O:83:LEU:HD11 | 22:O:115:LEU:HD22 | 2.01 | 0.42 |
| 22:O:7:ARG:HA | 22:O:10:ARG:NE | 2.34 | 0.42 |
| 2:B:1818:U:H2' | 4:C:152:GLN:O | 2.19 | 0.42 |
| 4:C:152:GLN:HA | 4:C:155:ARG:CD | 2.49 | 0.42 |
| 4:C:6:LYS:HA | 4:C:7:PRO:HD3 | 1.91 | 0.42 |
| 2:B:596:U:H2' | 2:B:597:G:C8 | 2.54 | 0.42 |
| 3:I:53:PRO:CG | 3:I:77:VAL:HG11 | 2.48 | 0.42 |
| 2:B:2352:A:N1 | 31:W:30:VAL:HG11 | 2.33 | 0.42 |
| 2:B:965:C:C2' | 2:B:966:G:H5' | 2.49 | 0.42 |
| 20:J:43:GLU:O | 20:J:44:TYR:C | 2.57 | 0.42 |
| 7:P:50:ARG:HD3 | 7:P:56:SER:HB3 | 1.99 | 0.42 |
| 27:G:122:ALA:HA | 27:G:131:VAL:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 2:B:1454:C:C5 | 21:N:64:ARG:HG2 | 2.54 | 0.42 |
| 21:N:79:LEU:O | 21:N:80:PHE:HB2 | 2.19 | 0.42 |
| 2:B:1439:A:N3 | 2:B:1553:A:C5 | 2.87 | 0.42 |
| 2:B:2032:G:H21 | 5:D:151:THR:H | 1.66 | 0.42 |
| 20:J:55:ILE:CG2 | 20:J:123:LYS:HB2 | 2.48 | 0.42 |
| 9:Y:8:GLN:HB3 | 9:Y:31:ILE:C | 2.40 | 0.42 |
| 2:B:335:C:OP2 | 25:U:81:ARG:NH1 | 2.51 | 0.42 |
| 9:Y:3:THR:HB | 9:Y:36:GLU:CG | 2.49 | 0.42 |
| 25:U:10:VAL:HB | 25:U:69:VAL:HB | 2.00 | 0.42 |
| 26:F:65:LEU:H | 26:F:88:VAL:HG22 | 1.84 | 0.42 |
| 2:B:2334:U:H5' | 22:O:12:THR:HB | 2.01 | 0.42 |
| 27:G:115:GLN:N | 27:G:115:GLN:CD | 2.72 | 0.42 |
| 2:B:246:C:C2' | 2:B:247:G:H5' | 2.49 | 0.42 |
| 2:B:2393:U:H5'' | 16:L:62:PRO:CG | 2.49 | 0.42 |
| 2:B:936:A:H2' | 2:B:937:C:C6 | 2.55 | 0.42 |
| 2:B:321:U:OP2 | 8:E:130:LYS:HA | 2.19 | 0.42 |
| 2:B:2601:C:O2' | 2:B:2602:A:H5'' | 2.18 | 0.42 |
| 1:A:92:C:O2' | 1:A:93:C:H5' | 2.19 | 0.42 |
| 27:G:108:PHE:C | 27:G:110:HIS:H | 2.22 | 0.42 |
| 2:B:588:U:H1' | 8:E:85:PHE:CD1 | 2.54 | 0.42 |
| 2:B:728:G:O2' | 2:B:730:A:H8 | 2.01 | 0.42 |
| 2:B:2877:G:O2' | 2:B:2878:U:H5' | 2.20 | 0.42 |
| 2:B:692:C:H2' | 2:B:693:A:C8 | 2.54 | 0.42 |
| 2:B:909:A:H2' | 2:B:912:C:C5 | 2.54 | 0.42 |
| 7:P:31:VAL:HG13 | 7:P:32:VAL:N | 2.34 | 0.42 |
| 2:B:960:A:C4' | 2:B:2457:U:H4' | 2.49 | 0.42 |
| 15:2:34:ARG:HH11 | 15:2:34:ARG:HG2 | 1.83 | 0.42 |
| 15:2:34:ARG:NH1 | 15:2:34:ARG:HG2 | 2.34 | 0.42 |
| 2:B:2619:C:H5' | 5:D:157:LYS:HG2 | 2.02 | 0.42 |
| 16:L:77:ILE:CD1 | 16:L:101:ILE:HD11 | 2.50 | 0.42 |
| 20:J:4:PHE:CG | 20:J:5:THR:N | 2.87 | 0.42 |
| 14:V:70:ILE:HD13 | 14:V:70:ILE:N | 2.35 | 0.42 |
| 17:M:38:ARG:NH1 | 17:M:38:ARG:HB3 | 2.34 | 0.42 |
| 17:M:38:ARG:HA | 17:M:98:PRO:HD3 | 2.01 | 0.42 |
| 29:T:42:GLU:O | 29:T:46:ALA:HB2 | 2.18 | 0.42 |
| 24:S:33:LEU:HA | 24:S:36:LEU:HD23 | 2.01 | 0.42 |
| 17:M:2:LEU:HD11 | 17:M:68:PHE:CE1 | 2.53 | 0.42 |
| 2:B:1438:U:N3 | 2:B:1552:A:N6 | 2.67 | 0.42 |
| 11:4:17:VAL:HG11 | 11:4:19:ARG:HE | 1.84 | 0.42 |
| 20:J:53:TYR:O | 20:J:55:ILE:HG23 | 2.18 | 0.42 |
| 19:H:140:ALA:O | 19:H:142:VAL:HG23 | 2.19 | 0.42 |
| 2:B:2590:A:H2' | 2:B:2591:C:C6 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 8:E:119:ILE:O | 8:E:187:VAL:HA | 2.20 | 0.42 |
| 5:D:114:LYS:HD2 | 5:D:116:LYS:HZ1 | 1.81 | 0.42 |
| 26:F:57:ALA:HB2 | 26:F:64:PRO:HD3 | 2.01 | 0.42 |
| 26:F:149:ARG:HA | 26:F:149:ARG:NH1 | 2.27 | 0.42 |
| 2:B:483:A:O2' | 25:U:56:GLY:N | 2.52 | 0.42 |
| 2:B:476:G:N2 | 2:B:479:A:O4' | 2.47 | 0.42 |
| 4:C:249:VAL:O | 4:C:250:GLN:C | 2.57 | 0.42 |
| 8:E:11:ALA:C | 8:E:12:LEU:HD22 | 2.39 | 0.42 |
| 2:B:2138:G:H2' | 2:B:2139:U:C6 | 2.54 | 0.42 |
| 2:B:1505:A:H2' | 2:B:1506:U:H6 | 1.83 | 0.42 |
| 6:K:11:ALA:HB3 | 6:K:85:VAL:CG2 | 2.49 | 0.42 |
| 2:B:2294:G:H2' | 2:B:2295:C:H6 | 1.83 | 0.42 |
| 2:B:1586:A:O5' | 2:B:1586:A:H8 | 2.02 | 0.42 |
| 4:C:66:PHE:CD1 | 4:C:66:PHE:N | 2.86 | 0.42 |
| 20:J:77:HIS:HD2 | 20:J:84:ILE:H | 1.65 | 0.42 |
| 3:I:140:GLU:H | 3:I:140:GLU:CD | 2.22 | 0.42 |
| 22:O:29:HIS:HB3 | 22:O:36:TYR:HB2 | 2.01 | 0.42 |
| 25:U:6:ARG:O | 25:U:24:VAL:HB | 2.19 | 0.42 |
| 2:B:1092:C:H2' | 2:B:1093:G:C5' | 2.49 | 0.42 |
| 2:B:1831:G:H2' | 2:B:1832:C:H6 | 1.85 | 0.42 |
| 2:B:2234:G:O2' | 2:B:2235:G:H5' | 2.19 | 0.42 |
| 11:4:22:VAL:HB | 11:4:24:ARG:HE | 1.85 | 0.42 |
| 7:P:33:GLU:HA | 7:P:33:GLU:OE1 | 2.18 | 0.42 |
| 2:B:2324:U:H3' | 2:B:2325:G:C5' | 2.50 | 0.42 |
| 4:C:108:GLY:C | 4:C:110:LYS:H | 2.22 | 0.42 |
| 4:C:69:ASN:HB3 | 4:C:70:LYS:H | 1.62 | 0.42 |
| 2:B:818:G:H4' | 2:B:838:C:O3' | 2.19 | 0.42 |
| 31:W:23:LYS:C | 31:W:66:VAL:HB | 2.40 | 0.42 |
| 27:G:25:ILE:O | 27:G:32:LEU:HA | 2.19 | 0.42 |
| 29:T:16:VAL:HA | 29:T:21:SER:HB3 | 2.01 | 0.42 |
| 2:B:1176:U:H6 | 2:B:1176:U:O5' | 2.02 | 0.42 |
| 7:P:4:ILE:CG2 | 7:P:5:LYS:H | 2.17 | 0.42 |
| 17:M:71:LYS:HB3 | 17:M:93:VAL:O | 2.19 | 0.42 |
| 26:F:104:THR:C | 26:F:105:ILE:HG13 | 2.40 | 0.42 |
| 26:F:91:ARG:O | 26:F:92:GLY:C | 2.58 | 0.42 |
| 30:Z:33:LEU:HA | 30:Z:51:VAL:O | 2.19 | 0.42 |
| 2:B:1252:G:H5'' | 35:B:3883:HOH:O | 2.19 | 0.42 |
| 2:B:2720:U:H2' | 2:B:2721:A:H8 | 1.85 | 0.42 |
| 25:U:51:LEU:HD22 | 25:U:52:ASN:OD1 | 2.19 | 0.42 |
| 2:B:247:G:H4' | 2:B:386:G:C5 | 2.55 | 0.42 |
| 4:C:123:ILE:HA | 4:C:191:LEU:HD13 | 2.00 | 0.42 |
| 2:B:394:C:C2' | 2:B:395:U:H5' | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 16:L:2:ARG:HG2 | 16:L:2:ARG:O | 2.20 | 0.42 |
| 21:N:17:ARG:O | 21:N:21:PHE:HB2 | 2.19 | 0.42 |
| 1:A:94:A:OP1 | 14:V:19:ARG:HD3 | 2.18 | 0.42 |
| 2:B:175:G:H2' | 2:B:176:A:C8 | 2.54 | 0.42 |
| 2:B:1799:G:H4' | 2:B:1800:C:O5' | 2.20 | 0.42 |
| 19:H:27:ARG:O | 19:H:28:ASN:ND2 | 2.52 | 0.42 |
| 2:B:2488:G:O2' | 2:B:2489:U:H5' | 2.20 | 0.42 |
| 2:B:960:A:H61 | 17:M:82:MET:HE1 | 1.85 | 0.42 |
| 29:T:36:LYS:HD3 | 29:T:36:LYS:O | 2.20 | 0.42 |
| 2:B:8:C:O2' | 2:B:9:G:H5' | 2.19 | 0.42 |
| 2:B:2088:A:H2' | 2:B:2089:C:C6 | 2.54 | 0.42 |
| 2:B:1706:C:O2' | 2:B:1757:A:H5' | 2.20 | 0.42 |
| 31:W:28:GLU:H | 31:W:31:LEU:HD11 | 1.85 | 0.42 |
| 31:W:36:ILE:HG21 | 31:W:42:THR:HG21 | 2.02 | 0.42 |
| 31:W:81:ILE:HG13 | 31:W:81:ILE:O | 2.19 | 0.42 |
| 21:N:38:LEU:HB3 | 21:N:39:PRO:CD | 2.40 | 0.42 |
| 8:E:157:LEU:HG | 8:E:169:VAL:HG11 | 2.01 | 0.42 |
| 27:G:77:GLY:HA3 | 27:G:135:ALA:O | 2.20 | 0.42 |
| 20:J:45:THR:H | 20:J:46:PRO:CD | 2.28 | 0.42 |
| 20:J:6:ALA:HB3 | 20:J:45:THR:CG2 | 2.48 | 0.42 |
| 23:Q:94:LEU:O | 23:Q:97:ILE:HG23 | 2.20 | 0.42 |
| 28:R:4:VAL:HG21 | 28:R:39:LEU:HG | 2.01 | 0.42 |
| 19:H:2:GLN:O | 19:H:3:VAL:O | 2.38 | 0.42 |
| 5:D:57:ALA:HA | 5:D:60:VAL:HG21 | 2.01 | 0.42 |
| 14:V:29:ILE:HD13 | 14:V:31:TYR:HE2 | 1.84 | 0.42 |
| 2:B:1181:U:H2' | 2:B:1182:G:C8 | 2.52 | 0.42 |
| 26:F:100:GLU:O | 26:F:104:THR:HB | 2.19 | 0.42 |
| 24:S:18:ARG:O | 24:S:22:ASP:OD1 | 2.37 | 0.42 |
| 2:B:1547:C:H2' | 2:B:1548:A:C8 | 2.54 | 0.42 |
| 8:E:61:ARG:HG3 | 8:E:61:ARG:HH21 | 1.85 | 0.42 |
| 2:B:144:A:H2' | 2:B:145:C:H6 | 1.84 | 0.42 |
| 2:B:327:G:H2' | 2:B:328:U:C6 | 2.54 | 0.42 |
| 27:G:94:ARG:HE | 27:G:94:ARG:C | 2.22 | 0.42 |
| 16:L:65:GLY:O | 16:L:66:PHE:CB | 2.65 | 0.42 |
| 5:D:113:SER:HB3 | 5:D:167:ASN:CA | 2.49 | 0.42 |
| 29:T:50:LEU:O | 29:T:52:GLU:N | 2.52 | 0.42 |
| 2:B:154:U:O2' | 2:B:155:A:H5' | 2.20 | 0.42 |
| 2:B:2734:A:H2' | 2:B:2735:G:C5' | 2.47 | 0.42 |
| 13:3:61:LEU:N | 13:3:62:PRO:HD3 | 2.34 | 0.42 |
| 20:J:84:ILE:HG23 | 20:J:84:ILE:O | 2.19 | 0.42 |
| 2:B:99:U:O4' | 2:B:99:U:O2 | 2.34 | 0.42 |
| 4:C:172:THR:HB | 4:C:182:LYS:HG2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 23:Q:49:ARG:HH11 | 23:Q:49:ARG:HG2 | 1.85 | 0.42 |
| 3:I:46:ASP:HA | 3:I:50:LYS:HE2 | 2.01 | 0.42 |
| 2:B:1076:C:O2' | 2:B:1077:A:H5' | 2.20 | 0.42 |
| 2:B:1711:A:O2' | 2:B:1712:U:H5' | 2.19 | 0.42 |
| 2:B:1541:C:O2' | 2:B:1542:U:H5' | 2.19 | 0.42 |
| 2:B:856:G:C1' | 31:W:23:LYS:HB3 | 2.40 | 0.42 |
| 4:C:141:HIS:HB3 | 4:C:190:THR:HG1 | 1.85 | 0.42 |
| 20:J:112:GLY:N | 20:J:113:PRO:HD2 | 2.29 | 0.42 |
| 23:Q:63:ARG:HA | 23:Q:66:ALA:HB3 | 2.01 | 0.42 |
| 29:T:57:VAL:CG2 | 29:T:58:VAL:H | 2.19 | 0.42 |
| 2:B:1171:G:H2' | 2:B:1172:C:C6 | 2.54 | 0.42 |
| 27:G:102:ILE:CD1 | 27:G:116:LEU:HD11 | 2.49 | 0.42 |
| 17:M:41:LEU:HB3 | 17:M:46:ILE:CG2 | 2.50 | 0.42 |
| 21:N:102:PHE:N | 21:N:109:PRO:HA | 2.25 | 0.42 |
| 25:U:82:VAL:HG12 | 25:U:83:GLY:O | 2.19 | 0.42 |
| 31:W:77:LYS:O | 31:W:78:PHE:HB2 | 2.18 | 0.42 |
| 2:B:1841:U:C2 | 2:B:1842:G:C8 | 3.07 | 0.42 |
| 2:B:2394:C:H2' | 2:B:2395:C:C6 | 2.54 | 0.42 |
| 2:B:2394:C:OP1 | 16:L:63:LYS:HG2 | 2.19 | 0.42 |
| 2:B:2025:C:H2' | 2:B:2026:U:H6 | 1.83 | 0.42 |
| 2:B:780:G:H2' | 2:B:782:A:N7 | 2.35 | 0.42 |
| 2:B:1573:G:C2' | 2:B:1574:C:H5' | 2.49 | 0.42 |
| 4:C:52:HIS:NE2 | 4:C:218:THR:HG23 | 2.35 | 0.42 |
| 2:B:1009:A:OP1 | 20:J:39:LYS:NZ | 2.53 | 0.42 |
| 2:B:2251:G:OP2 | 2:B:2251:G:H8 | 2.02 | 0.42 |
| 2:B:2083:G:H2' | 2:B:2084:C:H6 | 1.84 | 0.42 |
| 2:B:1357:C:H2' | 2:B:1358:G:C8 | 2.55 | 0.42 |
| 2:B:910:A:H2 | 2:B:2264:C:O2 | 2.02 | 0.42 |
| 2:B:1562:U:H2' | 2:B:1563:U:C6 | 2.54 | 0.42 |
| 2:B:919:U:H6 | 2:B:919:U:O5' | 2.02 | 0.42 |
| 31:W:39:GLN:NE2 | 31:W:43:LYS:HB2 | 2.35 | 0.42 |
| 25:U:90:LYS:O | 25:U:92:VAL:HG23 | 2.20 | 0.42 |
| 5:D:109:VAL:HG11 | 5:D:193:VAL:CB | 2.49 | 0.42 |
| 4:C:131:MET:CE | 4:C:187:CYS:HB2 | 2.49 | 0.42 |
| 29:T:14:PRO:HA | 29:T:32:LEU:HB2 | 2.01 | 0.42 |
| 4:C:64:VAL:HA | 4:C:102:TYR:HB3 | 2.02 | 0.42 |
| 11:4:2:LYS:CD | 11:4:4:ARG:HG3 | 2.50 | 0.42 |
| 23:Q:65:ASN:HD21 | 23:Q:69:ARG:NH1 | 2.02 | 0.42 |
| 8:E:58:LYS:HB2 | 8:E:60:TRP:CD1 | 2.54 | 0.42 |
| 2:B:627:A:P | 16:L:78:ARG:HH11 | 2.42 | 0.42 |
| 3:I:12:VAL:HG13 | 3:I:41:PHE:CE2 | 2.55 | 0.42 |
| 8:E:51:GLU:H | 8:E:51:GLU:HG2 | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-------------------|-------------|----------|
| 2:B:581:C:OP2 | 23:Q:32:ARG:HD2 | 2.19 | 0.42 |
| 2:B:581:C:P | 23:Q:32:ARG:HD2 | 2.59 | 0.42 |
| 2:B:193:U:O3' | 2:B:803:U:H4' | 2.20 | 0.42 |
| 4:C:257:ARG:HG3 | 4:C:257:ARG:HH11 | 1.84 | 0.42 |
| 2:B:654:A:H2' | 2:B:655:A:C5' | 2.49 | 0.42 |
| 2:B:1411:U:H2' | 2:B:1412:U:H6 | 1.84 | 0.42 |
| 2:B:315:G:H2' | 2:B:316:C:H6 | 1.80 | 0.42 |
| 22:O:110:ALA:O | 22:O:115:LEU:HB2 | 2.20 | 0.42 |
| 2:B:2185:U:H2' | 2:B:2186:G:O4' | 2.20 | 0.42 |
| 2:B:1317:G:H2' | 2:B:1318:U:O4' | 2.20 | 0.42 |
| 2:B:730:A:O2' | 2:B:731:C:H5' | 2.20 | 0.42 |
| 8:E:111:GLU:HA | 8:E:114:ARG:CZ | 2.50 | 0.42 |
| 2:B:1266:G:OP1 | 10:O:15:ARG:NE | 2.49 | 0.42 |
| 2:B:2397:G:O2' | 2:B:2398:U:H5' | 2.20 | 0.42 |
| 2:B:226:A:H2' | 2:B:227:A:C8 | 2.54 | 0.42 |
| 2:B:499:U:H2' | 2:B:500:G:O4' | 2.18 | 0.42 |
| 2:B:84:A:H4' | 2:B:85:G:O5' | 2.20 | 0.42 |
| 2:B:2508:G:H2' | 2:B:2509:G:H8 | 1.84 | 0.42 |
| 3:I:68:PHE:N | 3:I:68:PHE:CD1 | 2.88 | 0.42 |
| 2:B:406:G:O2' | 2:B:407:G:H5' | 2.19 | 0.42 |
| 2:B:1893:C:H2' | 2:B:1894:C:O4' | 2.19 | 0.42 |
| 2:B:1666:G:O2' | 2:B:1667:G:H5' | 2.19 | 0.42 |
| 27:G:17:LYS:HG3 | 27:G:18:ILE:N | 2.34 | 0.42 |
| 27:G:28:LYS:O | 27:G:29:ASN:HB3 | 2.19 | 0.42 |
| 20:J:41:LYS:O | 23:Q:66:ALA:HB1 | 2.20 | 0.42 |
| 7:P:3:ILE:CD1 | 7:P:7:LEU:HD11 | 2.50 | 0.42 |
| 27:G:84:LYS:O | 27:G:85:LYS:O | 2.38 | 0.42 |
| 24:S:18:ARG:NH2 | 24:S:76:VAL:O | 2.53 | 0.42 |
| 2:B:544:C:H2' | 2:B:545:U:C6 | 2.54 | 0.42 |
| 6:K:42:THR:O | 6:K:44:LYS:HG2 | 2.20 | 0.42 |
| 2:B:1338:G:O2' | 2:B:1393:A:N1 | 2.47 | 0.42 |
| 2:B:1140:C:C2' | 2:B:1141:U:H5' | 2.50 | 0.42 |
| 2:B:2144:G:N2 | 2:B:2146:C:O4' | 2.52 | 0.42 |
| 27:G:94:ARG:CB | 27:G:127:GLN:HG2 | 2.49 | 0.42 |
| 25:U:95:PHE:HZ | 25:U:102:ILE:HD13 | 1.85 | 0.42 |
| 17:M:21:ALA:HB1 | 17:M:100:LYS:HG2 | 2.01 | 0.42 |
| 8:E:134:LEU:CD2 | 8:E:161:ALA:HB2 | 2.50 | 0.42 |
| 2:B:484:C:H2' | 2:B:485:C:H6 | 1.84 | 0.42 |
| 2:B:485:C:H2' | 2:B:486:C:H6 | 1.85 | 0.42 |
| 2:B:2893:A:H4' | 2:B:2894:G:C5' | 2.50 | 0.42 |
| 2:B:231:A:H3' | 2:B:232:G:H8 | 1.84 | 0.42 |
| 6:K:61:VAL:HG23 | 6:K:61:VAL:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:839:U:H2' | 2:B:840:C:H6 | 1.85 | 0.42 |
| 7:P:99:LEU:HD13 | 7:P:102:ARG:HG3 | 2.02 | 0.42 |
| 22:O:51:ALA:HB3 | 22:O:78:VAL:HG13 | 2.01 | 0.42 |
| 21:N:17:ARG:C | 21:N:19:ALA:N | 2.72 | 0.42 |
| 2:B:2693:G:H2' | 2:B:2694:G:H8 | 1.84 | 0.42 |
| 2:B:2407:A:H2' | 2:B:2408:U:C6 | 2.53 | 0.42 |
| 2:B:730:A:C2 | 2:B:731:C:C6 | 3.07 | 0.42 |
| 2:B:2077:A:C5 | 2:B:2435:A:C5 | 3.08 | 0.42 |
| 2:B:2405:G:H2' | 2:B:2411:A:N6 | 2.34 | 0.42 |
| 2:B:2617:U:C2' | 2:B:2618:G:H5' | 2.49 | 0.42 |
| 7:P:28:LYS:HD2 | 7:P:82:SER:CB | 2.50 | 0.42 |
| 2:B:2219:U:O2' | 2:B:2220:U:H5' | 2.19 | 0.42 |
| 4:C:154:ALA:HB2 | 4:C:161:VAL:HG23 | 2.00 | 0.42 |
| 2:B:1062:G:H2' | 2:B:1063:G:H8 | 1.84 | 0.42 |
| 2:B:1987:A:H2' | 2:B:1988:G:C8 | 2.55 | 0.42 |
| 2:B:1541:C:H2' | 2:B:1542:U:H6 | 1.85 | 0.42 |
| 2:B:409:G:H2' | 2:B:410:G:C8 | 2.55 | 0.42 |
| 20:J:78:THR:HG21 | 20:J:85:LYS:HE2 | 2.02 | 0.42 |
| 27:G:44:HIS:O | 27:G:46:ASP:N | 2.53 | 0.42 |
| 23:Q:84:LYS:O | 23:Q:86:SER:N | 2.53 | 0.42 |
| 23:Q:89:ILE:HB | 23:Q:90:ASP:H | 1.72 | 0.42 |
| 29:T:57:VAL:O | 29:T:85:VAL:O | 2.37 | 0.42 |
| 11:4:2:LYS:O | 11:4:35:GLN:HA | 2.19 | 0.42 |
| 27:G:120:ILE:HD13 | 27:G:120:ILE:C | 2.40 | 0.42 |
| 30:Z:33:LEU:O | 30:Z:34:HIS:CG | 2.73 | 0.42 |
| 16:L:80:SER:H | 16:L:113:ALA:HB3 | 1.84 | 0.42 |
| 16:L:79:LEU:CB | 16:L:113:ALA:H | 2.31 | 0.42 |
| 3:I:41:PHE:CE2 | 3:I:45:THR:HG21 | 2.55 | 0.42 |
| 25:U:35:VAL:O | 25:U:38:ILE:HG22 | 2.20 | 0.42 |
| 2:B:433:C:H2' | 2:B:434:U:C6 | 2.54 | 0.42 |
| 13:3:31:ILE:HD11 | 13:3:34:LYS:CE | 2.50 | 0.42 |
| 2:B:245:G:H2' | 2:B:246:C:H6 | 1.85 | 0.42 |
| 2:B:2742:G:OP1 | 11:4:36:ARG:HD2 | 2.19 | 0.42 |
| 17:M:114:ARG:HG3 | 17:M:130:PHE:CD2 | 2.54 | 0.42 |
| 8:E:192:ALA:HA | 8:E:195:GLN:NE2 | 2.35 | 0.42 |
| 18:X:59:GLU:H | 18:X:59:GLU:CD | 2.23 | 0.42 |
| 2:B:587:C:H4' | 2:B:588:U:C6 | 2.55 | 0.42 |
| 2:B:600:G:H2' | 2:B:601:C:C6 | 2.55 | 0.42 |
| 2:B:2685:G:O2' | 2:B:2686:G:H5' | 2.20 | 0.42 |
| 2:B:2523:G:O2' | 2:B:2524:G:H5' | 2.20 | 0.42 |
| 2:B:1653:G:O6 | 21:N:10:LEU:O | 2.37 | 0.42 |
| 2:B:571:U:H1' | 2:B:573:U:C6 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:198:C:H2' | 2:B:199:A:H5'' | 2.01 | 0.42 |
| 16:L:122:VAL:HG23 | 16:L:143:GLU:OE1 | 2.20 | 0.42 |
| 2:B:996:A:H4' | 23:Q:91:ARG:CD | 2.49 | 0.42 |
| 20:J:38:GLY:CA | 20:J:51:GLY:HA2 | 2.50 | 0.42 |
| 23:Q:73:ILE:HD11 | 23:Q:77:LYS:CB | 2.48 | 0.42 |
| 2:B:1179:G:O2' | 2:B:1180:U:H5' | 2.20 | 0.42 |
| 1:A:43:C:C2' | 1:A:44:G:H5'' | 2.50 | 0.42 |
| 2:B:1287:A:P | 21:N:104:ALA:HB3 | 2.58 | 0.42 |
| 22:O:18:LEU:HD23 | 22:O:25:ARG:CD | 2.50 | 0.42 |
| 22:O:25:ARG:HD2 | 22:O:93:ASP:HB2 | 2.02 | 0.42 |
| 19:H:112:LYS:HA | 19:H:132:PHE:HE1 | 1.84 | 0.42 |
| 27:G:104:LEU:O | 27:G:112:VAL:N | 2.53 | 0.42 |
| 27:G:167:VAL:HG23 | 27:G:168:VAL:N | 2.32 | 0.42 |
| 17:M:66:ARG:NE | 17:M:101:VAL:HG11 | 2.35 | 0.42 |
| 13:3:33:THR:HG23 | 13:3:34:LYS:N | 2.34 | 0.42 |
| 23:Q:28:SER:C | 23:Q:29:ARG:HG3 | 2.41 | 0.42 |
| 6:K:110:GLU:HA | 6:K:113:MET:CG | 2.50 | 0.42 |
| 2:B:631:A:O2' | 16:L:66:PHE:HD2 | 1.96 | 0.42 |
| 2:B:2801:G:H3' | 2:B:2802:G:H8 | 1.83 | 0.42 |
| 2:B:1300:G:H4' | 2:B:1301:A:O5' | 2.20 | 0.42 |
| 20:J:37:ARG:HH22 | 20:J:110:PRO:HG3 | 1.82 | 0.42 |
| 20:J:31:GLU:OE2 | 20:J:31:GLU:HA | 2.19 | 0.42 |
| 2:B:2023:C:O2' | 2:B:2024:G:H5' | 2.20 | 0.42 |
| 2:B:978:G:O4' | 2:B:1001:A:H2 | 2.02 | 0.42 |
| 2:B:623:C:H2' | 2:B:624:C:H6 | 1.85 | 0.42 |
| 2:B:131:A:H2' | 2:B:132:G:C8 | 2.54 | 0.42 |
| 6:K:25:LEU:CD1 | 6:K:38:ILE:HG22 | 2.50 | 0.42 |
| 2:B:104:A:H2' | 2:B:105:C:C6 | 2.55 | 0.42 |
| 24:S:3:THR:O | 24:S:3:THR:HG23 | 2.20 | 0.42 |
| 2:B:2651:C:H2' | 2:B:2652:C:H6 | 1.84 | 0.42 |
| 2:B:1596:A:O2' | 2:B:1597:A:H5' | 2.20 | 0.42 |
| 2:B:2613:U:H5'' | 35:B:4016:HOH:O | 2.20 | 0.42 |
| 2:B:1326:U:H2' | 2:B:1327:A:H8 | 1.83 | 0.42 |
| 2:B:923:G:H1' | 31:W:23:LYS:HZ1 | 1.84 | 0.41 |
| 4:C:43:ASN:ND2 | 4:C:44:ASN:H | 2.18 | 0.41 |
| 19:H:3:VAL:CG1 | 19:H:38:PRO:HA | 2.50 | 0.41 |
| 19:H:122:LEU:C | 19:H:124:THR:H | 2.23 | 0.41 |
| 19:H:94:ILE:HA | 19:H:94:ILE:HD12 | 1.84 | 0.41 |
| 7:P:75:THR:CG2 | 7:P:76:HIS:H | 2.24 | 0.41 |
| 23:Q:7:VAL:CG2 | 23:Q:8:ILE:N | 2.82 | 0.41 |
| 27:G:120:ILE:HG13 | 27:G:140:ILE:HG22 | 2.02 | 0.41 |
| 21:N:55:ALA:HA | 21:N:80:PHE:CD1 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 21:N:63:ARG:HA | 21:N:80:PHE:CE2 | 2.55 | 0.41 |
| 24:S:48:LYS:HE2 | 24:S:52:GLU:OE1 | 2.20 | 0.41 |
| 30:Z:32:ASN:HB3 | 30:Z:53:ALA:H | 1.85 | 0.41 |
| 19:H:97:ARG:HA | 19:H:112:LYS:HD3 | 2.02 | 0.41 |
| 4:C:94:LEU:HG | 4:C:94:LEU:O | 2.19 | 0.41 |
| 2:B:435:C:H2' | 2:B:436:C:H5' | 2.02 | 0.41 |
| 7:P:97:TYR:O | 7:P:100:ARG:HD3 | 2.20 | 0.41 |
| 2:B:1348:C:C3' | 2:B:1349:C:H5' | 2.50 | 0.41 |
| 2:B:1720:U:O2' | 2:B:1721:G:H5' | 2.20 | 0.41 |
| 2:B:1508:A:H5' | 2:B:1509:A:N7 | 2.35 | 0.41 |
| 2:B:1511:G:H2' | 2:B:1512:C:C6 | 2.55 | 0.41 |
| 5:D:124:ARG:O | 5:D:124:ARG:HG3 | 2.19 | 0.41 |
| 2:B:2024:G:H2' | 2:B:2025:C:O4' | 2.20 | 0.41 |
| 3:I:99:LYS:HB2 | 3:I:140:GLU:OE1 | 2.19 | 0.41 |
| 2:B:1641:A:H2' | 2:B:1642:G:O4' | 2.20 | 0.41 |
| 27:G:72:ASN:O | 27:G:75:VAL:HB | 2.20 | 0.41 |
| 2:B:2348:U:OP1 | 13:3:37:THR:HG21 | 2.19 | 0.41 |
| 2:B:2780:G:H4' | 2:B:2781:A:OP2 | 2.19 | 0.41 |
| 2:B:1712:U:H2' | 2:B:1713:A:N7 | 2.35 | 0.41 |
| 3:I:91:LYS:N | 3:I:91:LYS:HD2 | 2.34 | 0.41 |
| 2:B:2428:G:H5'' | 2:B:2429:G:OP1 | 2.20 | 0.41 |
| 2:B:120:U:H5'' | 2:B:122:G:OP2 | 2.19 | 0.41 |
| 2:B:1097:U:C2 | 2:B:1098:A:H1' | 2.56 | 0.41 |
| 27:G:26:LYS:HG2 | 27:G:27:GLY:N | 2.35 | 0.41 |
| 27:G:42:VAL:HG23 | 27:G:49:LEU:HB3 | 2.02 | 0.41 |
| 27:G:74:MET:O | 27:G:78:VAL:HG22 | 2.20 | 0.41 |
| 19:H:88:GLY:C | 19:H:124:THR:HA | 2.40 | 0.41 |
| 14:V:28:ALA:CB | 14:V:89:ILE:HD12 | 2.48 | 0.41 |
| 27:G:84:LYS:CG | 27:G:85:LYS:H | 2.16 | 0.41 |
| 17:M:124:LEU:HA | 17:M:125:PRO:HD3 | 1.88 | 0.41 |
| 26:F:96:TRP:O | 26:F:100:GLU:N | 2.53 | 0.41 |
| 2:B:362:A:H2' | 2:B:363:G:O4' | 2.20 | 0.41 |
| 2:B:1021:A:H61 | 2:B:1142:A:H61 | 1.68 | 0.41 |
| 4:C:78:GLU:HG3 | 4:C:94:LEU:HB3 | 2.02 | 0.41 |
| 10:O:42:ILE:HG22 | 10:O:43:THR:O | 2.19 | 0.41 |
| 2:B:2799:A:H4' | 2:B:2800:A:C1' | 2.49 | 0.41 |
| 14:V:62:THR:HG22 | 14:V:71:LYS:HZ3 | 1.85 | 0.41 |
| 2:B:478:A:H5'' | 2:B:479:A:OP2 | 2.20 | 0.41 |
| 2:B:1902:C:H4' | 4:C:241:LYS:O | 2.19 | 0.41 |
| 13:3:21:PHE:O | 13:3:22:LYS:HB3 | 2.20 | 0.41 |
| 2:B:62:U:H2' | 2:B:63:A:O4' | 2.20 | 0.41 |
| 29:T:50:LEU:O | 29:T:51:PHE:HB2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 22:O:54:VAL:HG13 | 22:O:55:GLU:N | 2.35 | 0.41 |
| 16:L:21:ARG:HD3 | 16:L:21:ARG:HA | 1.83 | 0.41 |
| 2:B:2776:A:H4' | 2:B:2777:G:O5' | 2.21 | 0.41 |
| 2:B:739:A:H1' | 2:B:740:C:H5 | 1.83 | 0.41 |
| 2:B:629:G:OP1 | 2:B:650:C:O2' | 2.37 | 0.41 |
| 2:B:1637:A:H2' | 2:B:1638:C:C6 | 2.55 | 0.41 |
| 25:U:48:VAL:O | 25:U:50:ALA:N | 2.53 | 0.41 |
| 2:B:217:A:H2' | 2:B:218:A:O4' | 2.20 | 0.41 |
| 2:B:1649:G:HO2' | 2:B:1650:A:H5' | 1.85 | 0.41 |
| 2:B:1541:C:H2' | 2:B:1542:U:C6 | 2.54 | 0.41 |
| 16:L:41:ARG:HH21 | 16:L:41:ARG:HG2 | 1.85 | 0.41 |
| 2:B:1207:C:H2' | 2:B:1208:C:H6 | 1.84 | 0.41 |
| 8:E:171:ASP:CG | 8:E:172:ALA:N | 2.73 | 0.41 |
| 2:B:695:G:OP1 | 2:B:1380:G:H4' | 2.20 | 0.41 |
| 2:B:2363:G:O2' | 2:B:2364:C:H5' | 2.19 | 0.41 |
| 2:B:1249:U:O4' | 23:Q:3:VAL:HG21 | 2.19 | 0.41 |
| 2:B:1068:G:C6 | 2:B:1069:A:N6 | 2.88 | 0.41 |
| 2:B:920:A:H2' | 2:B:921:C:H6 | 1.85 | 0.41 |
| 3:I:131:THR:O | 3:I:135:MET:HG3 | 2.19 | 0.41 |
| 28:R:8:GLY:CA | 28:R:23:GLU:HB2 | 2.37 | 0.41 |
| 2:B:1252:G:H1 | 23:Q:36:GLN:CD | 2.23 | 0.41 |
| 12:I:20:TYR:CD2 | 12:I:37:LYS:HD3 | 2.56 | 0.41 |
| 25:U:65:GLN:HB2 | 25:U:68:ASN:HD22 | 1.86 | 0.41 |
| 22:O:47:VAL:HG12 | 22:O:48:LEU:N | 2.35 | 0.41 |
| 2:B:2733:A:H8 | 2:B:2733:A:O5' | 2.03 | 0.41 |
| 21:N:49:GLU:HA | 21:N:94:TYR:HD2 | 1.85 | 0.41 |
| 25:U:21:ARG:HD3 | 25:U:72:PHE:CG | 2.54 | 0.41 |
| 2:B:1346:G:HO2' | 2:B:1347:A:H5' | 1.84 | 0.41 |
| 2:B:992:C:H2' | 2:B:993:G:H8 | 1.86 | 0.41 |
| 5:D:169:ARG:O | 5:D:170:VAL:O | 2.37 | 0.41 |
| 4:C:30:ALA:C | 4:C:32:LEU:H | 2.23 | 0.41 |
| 2:B:1494:A:H2' | 2:B:1495:A:H8 | 1.83 | 0.41 |
| 3:I:5:GLN:O | 3:I:6:ALA:CB | 2.68 | 0.41 |
| 2:B:2093:G:O2' | 2:B:2094:A:H5' | 2.21 | 0.41 |
| 2:B:2097:A:H2' | 2:B:2098:U:C6 | 2.55 | 0.41 |
| 2:B:2852:G:H2' | 2:B:2853:C:C6 | 2.55 | 0.41 |
| 4:C:162:GLN:CD | 4:C:174:ARG:HH21 | 2.23 | 0.41 |
| 10:O:55:ALA:C | 10:O:56:LYS:HG3 | 2.41 | 0.41 |
| 2:B:2716:C:O2' | 2:B:2717:C:H5' | 2.20 | 0.41 |
| 2:B:1628:G:O2' | 2:B:1629:U:H5' | 2.19 | 0.41 |
| 2:B:1651:G:H2' | 2:B:1652:A:O4' | 2.20 | 0.41 |
| 2:B:1812:U:O2' | 4:C:43:ASN:ND2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:P:3:ILE:HG23 | 7:P:4:ILE:HG13 | 2.02 | 0.41 |
| 4:C:109:LEU:H | 4:C:109:LEU:HD23 | 1.84 | 0.41 |
| 11:4:8:LYS:HE2 | 11:4:8:LYS:HB3 | 1.91 | 0.41 |
| 24:S:50:VAL:HA | 24:S:53:SER:HB2 | 2.03 | 0.41 |
| 26:F:27:VAL:O | 26:F:27:VAL:HG23 | 2.21 | 0.41 |
| 10:0:27:LEU:HB2 | 10:0:28:SER:H | 1.61 | 0.41 |
| 2:B:675:A:P | 8:E:60:TRP:HZ2 | 2.43 | 0.41 |
| 2:B:2378:A:N3 | 22:O:18:LEU:HD13 | 2.34 | 0.41 |
| 19:H:131:SER:OG | 19:H:132:PHE:N | 2.51 | 0.41 |
| 27:G:87:GLN:HG3 | 27:G:128:THR:O | 2.21 | 0.41 |
| 6:K:99:ILE:H | 6:K:118:LEU:HD22 | 1.85 | 0.41 |
| 2:B:2049:G:O2' | 2:B:2050:C:H5' | 2.20 | 0.41 |
| 28:R:15:SER:HB3 | 28:R:18:GLN:HE21 | 1.85 | 0.41 |
| 17:M:57:VAL:HG12 | 17:M:60:GLN:O | 2.20 | 0.41 |
| 2:B:244:A:H2' | 2:B:245:G:O4' | 2.21 | 0.41 |
| 26:F:45:ASP:OD1 | 26:F:47:LYS:HB2 | 2.21 | 0.41 |
| 2:B:876:C:H2' | 2:B:877:A:O4' | 2.20 | 0.41 |
| 2:B:967:U:H2' | 2:B:968:C:H6 | 1.83 | 0.41 |
| 2:B:1668:A:O2' | 2:B:1674:G:N7 | 2.44 | 0.41 |
| 2:B:2309:A:H61 | 26:F:75:GLY:CA | 2.34 | 0.41 |
| 6:K:109:SER:O | 6:K:111:LYS:N | 2.53 | 0.41 |
| 2:B:1526:C:O2' | 2:B:1527:G:H5' | 2.21 | 0.41 |
| 24:S:70:LYS:HD3 | 24:S:110:ARG:C | 2.40 | 0.41 |
| 31:W:54:ARG:HB2 | 31:W:54:ARG:HH11 | 1.86 | 0.41 |
| 2:B:991:C:H5' | 2:B:991:C:H6 | 1.85 | 0.41 |
| 29:T:6:ARG:HB3 | 29:T:6:ARG:NH1 | 2.36 | 0.41 |
| 8:E:173:THR:C | 8:E:175:ILE:H | 2.22 | 0.41 |
| 2:B:977:G:H4' | 2:B:1155:A:H5' | 2.02 | 0.41 |
| 2:B:560:C:H2' | 2:B:561:G:O4' | 2.20 | 0.41 |
| 23:Q:97:ILE:HD11 | 23:Q:108:LEU:CD1 | 2.51 | 0.41 |
| 4:C:91:ALA:N | 4:C:103:ILE:O | 2.53 | 0.41 |
| 29:T:69:ARG:NE | 29:T:70:HIS:H | 2.13 | 0.41 |
| 3:I:72:THR:HG23 | 3:I:112:LYS:HD2 | 2.02 | 0.41 |
| 2:B:279:A:N6 | 2:B:280:U:O2 | 2.53 | 0.41 |
| 26:F:34:THR:O | 26:F:35:LEU:HB2 | 2.20 | 0.41 |
| 26:F:95:MET:O | 26:F:98:PHE:HB3 | 2.20 | 0.41 |
| 2:B:2527:C:O2' | 2:B:2528:U:H5' | 2.21 | 0.41 |
| 5:D:48:ILE:HD12 | 5:D:89:GLU:HG2 | 2.02 | 0.41 |
| 6:K:43:ILE:CG2 | 6:K:54:LYS:HA | 2.50 | 0.41 |
| 2:B:135:U:H2' | 2:B:136:G:C8 | 2.55 | 0.41 |
| 9:Y:7:THR:HG22 | 9:Y:8:GLN:N | 2.35 | 0.41 |
| 21:N:48:VAL:O | 21:N:51:LEU:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:I:129:GLU:O | 3:I:133:ARG:HG3 | 2.20 | 0.41 |
| 26:F:87:LYS:C | 26:F:88:VAL:HG23 | 2.41 | 0.41 |
| 2:B:593:U:H2' | 2:B:594:U:C6 | 2.55 | 0.41 |
| 7:P:61:ARG:CB | 7:P:61:ARG:HH21 | 2.29 | 0.41 |
| 2:B:1842:G:H2' | 2:B:1843:C:C6 | 2.55 | 0.41 |
| 4:C:250:GLN:CG | 4:C:254:LYS:HG2 | 2.50 | 0.41 |
| 2:B:2815:C:H2' | 2:B:2816:G:C8 | 2.56 | 0.41 |
| 22:O:94:ARG:O | 22:O:97:PHE:HB2 | 2.21 | 0.41 |
| 6:K:107:LEU:C | 6:K:109:SER:H | 2.22 | 0.41 |
| 2:B:1997:C:O2' | 2:B:1998:A:H5' | 2.21 | 0.41 |
| 2:B:572:A:C2 | 2:B:2033:A:C2 | 3.09 | 0.41 |
| 2:B:2022:U:O2' | 2:B:2617:U:H5' | 2.21 | 0.41 |
| 2:B:464:U:C2 | 2:B:788:A:C6 | 3.09 | 0.41 |
| 2:B:2016:U:H2' | 2:B:2017:U:C6 | 2.56 | 0.41 |
| 10:O:35:GLU:HG3 | 10:O:45:ASP:OD1 | 2.20 | 0.41 |
| 27:G:155:PRO:HA | 27:G:170:THR:HA | 2.02 | 0.41 |
| 2:B:596:U:H2' | 2:B:597:G:H8 | 1.85 | 0.41 |
| 8:E:105:LEU:HA | 8:E:105:LEU:HD23 | 1.90 | 0.41 |
| 27:G:139:VAL:O | 27:G:142:GLN:HB3 | 2.21 | 0.41 |
| 2:B:2283:C:H2' | 2:B:2284:A:H5' | 2.03 | 0.41 |
| 31:W:30:VAL:HG21 | 31:W:59:PHE:CE1 | 2.56 | 0.41 |
| 5:D:107:VAL:HA | 5:D:204:LYS:O | 2.19 | 0.41 |
| 4:C:67:LYS:O | 4:C:188:ARG:HD3 | 2.20 | 0.41 |
| 20:J:44:TYR:O | 20:J:45:THR:CB | 2.67 | 0.41 |
| 23:Q:87:VAL:HG12 | 23:Q:89:ILE:HD13 | 2.02 | 0.41 |
| 19:H:95:GLY:N | 19:H:98:ASP:OD2 | 2.53 | 0.41 |
| 17:M:19:GLY:CA | 17:M:38:ARG:HH22 | 2.33 | 0.41 |
| 17:M:1:MET:HG2 | 17:M:2:LEU:N | 2.35 | 0.41 |
| 6:K:19:VAL:HG23 | 6:K:41:ILE:HD11 | 2.02 | 0.41 |
| 2:B:1082:U:H2' | 2:B:1083:U:O4' | 2.21 | 0.41 |
| 2:B:1022:G:N2 | 2:B:1142:A:C2 | 2.84 | 0.41 |
| 2:B:2733:A:C3' | 2:B:2733:A:C8 | 3.04 | 0.41 |
| 2:B:627:A:H4' | 2:B:628:G:OP1 | 2.20 | 0.41 |
| 27:G:88:LEU:HD11 | 27:G:94:ARG:N | 2.35 | 0.41 |
| 2:B:2811:G:O2' | 2:B:2812:G:H5' | 2.21 | 0.41 |
| 8:E:51:GLU:OE2 | 8:E:88:ARG:NH1 | 2.53 | 0.41 |
| 2:B:2723:C:O3' | 21:N:1:MET:HE1 | 2.20 | 0.41 |
| 2:B:1785:A:H2' | 2:B:1787:A:C8 | 2.54 | 0.41 |
| 4:C:196:ASN:C | 4:C:198:GLU:H | 2.23 | 0.41 |
| 2:B:1726:C:H2' | 2:B:1727:C:H6 | 1.80 | 0.41 |
| 2:B:1790:C:H2' | 2:B:1791:A:C8 | 2.55 | 0.41 |
| 18:X:44:LYS:HZ3 | 18:X:48:ARG:CZ | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 26:F:177:ARG:NE | 26:F:177:ARG:HA | 2.34 | 0.41 |
| 2:B:635:C:O2' | 2:B:639:U:OP1 | 2.37 | 0.41 |
| 2:B:878:A:H5' | 2:B:900:A:N6 | 2.33 | 0.41 |
| 2:B:114:U:H2' | 2:B:115:C:C6 | 2.55 | 0.41 |
| 22:O:83:LEU:CD1 | 22:O:115:LEU:HD22 | 2.51 | 0.41 |
| 30:Z:45:ARG:HE | 30:Z:47:VAL:CG1 | 2.34 | 0.41 |
| 2:B:866:A:H61 | 2:B:913:U:C1' | 2.32 | 0.41 |
| 2:B:2568:U:H2' | 2:B:2569:G:O4' | 2.21 | 0.41 |
| 30:Z:21:ALA:HB3 | 30:Z:23:ASN:ND2 | 2.36 | 0.41 |
| 8:E:37:ALA:C | 8:E:39:ALA:H | 2.22 | 0.41 |
| 2:B:2323:G:C2' | 2:B:2324:U:H5' | 2.51 | 0.41 |
| 2:B:1669:A:H2' | 2:B:1669:A:N3 | 2.35 | 0.41 |
| 2:B:1306:C:H2' | 2:B:1307:A:H8 | 1.85 | 0.41 |
| 4:C:136:VAL:HG12 | 4:C:137:GLY:N | 2.36 | 0.41 |
| 2:B:2336:A:O2' | 2:B:2337:G:O5' | 2.39 | 0.41 |
| 2:B:2370:G:H2' | 2:B:2371:G:O4' | 2.21 | 0.41 |
| 16:L:90:VAL:CB | 16:L:122:VAL:HG12 | 2.47 | 0.41 |
| 29:T:21:SER:HB3 | 29:T:31:VAL:CG2 | 2.51 | 0.41 |
| 29:T:25:GLU:OE1 | 29:T:30:ILE:HG13 | 2.20 | 0.41 |
| 3:I:73:PRO:CG | 3:I:78:LEU:HD21 | 2.47 | 0.41 |
| 26:F:111:ARG:CD | 26:F:111:ARG:N | 2.84 | 0.41 |
| 26:F:137:PHE:O | 26:F:138:PRO:C | 2.59 | 0.41 |
| 26:F:31:GLU:O | 26:F:31:GLU:HG3 | 2.21 | 0.41 |
| 19:H:10:ALA:O | 19:H:12:LEU:N | 2.50 | 0.41 |
| 2:B:2071:A:H2' | 2:B:2072:C:H6 | 1.82 | 0.41 |
| 31:W:8:SER:N | 31:W:10:ARG:HH12 | 2.17 | 0.41 |
| 16:L:79:LEU:HB3 | 16:L:115:GLU:H | 1.85 | 0.41 |
| 19:H:116:ARG:HB2 | 19:H:133:GLN:HE22 | 1.86 | 0.41 |
| 6:K:75:SER:HA | 7:P:72:VAL:O | 2.20 | 0.41 |
| 2:B:873:C:H2' | 2:B:874:G:O4' | 2.21 | 0.41 |
| 23:Q:26:ALA:HA | 23:Q:29:ARG:HD2 | 2.03 | 0.41 |
| 2:B:2680:U:H5' | 5:D:194:PRO:HA | 2.03 | 0.41 |
| 26:F:65:LEU:O | 26:F:86:CYS:HA | 2.21 | 0.41 |
| 8:E:170:ARG:HG2 | 8:E:174:GLY:O | 2.21 | 0.41 |
| 2:B:63:A:H5'' | 2:B:64:A:OP1 | 2.21 | 0.41 |
| 2:B:1347:A:H2' | 2:B:1348:C:O4' | 2.20 | 0.41 |
| 14:V:80:HIS:CD2 | 14:V:81:PRO:HD2 | 2.55 | 0.41 |
| 8:E:68:ALA:O | 8:E:69:ARG:C | 2.59 | 0.41 |
| 21:N:12:ARG:HG2 | 21:N:16:HIS:ND1 | 2.36 | 0.41 |
| 2:B:1683:U:O2' | 2:B:1684:G:H5' | 2.21 | 0.41 |
| 2:B:2075:U:H2' | 2:B:2077:A:OP1 | 2.21 | 0.41 |
| 2:B:572:A:C5' | 28:R:80:ARG:HH22 | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 6:K:88:ASN:ND2 | 6:K:88:ASN:C | 2.73 | 0.41 |
| 2:B:1389:G:O2' | 2:B:1390:U:H5' | 2.21 | 0.41 |
| 1:A:17:C:O2' | 1:A:18:G:H5' | 2.20 | 0.41 |
| 2:B:121:G:H2' | 2:B:122:G:C8 | 2.56 | 0.41 |
| 31:W:50:VAL:O | 31:W:52:CYS:N | 2.53 | 0.41 |
| 21:N:38:LEU:CB | 21:N:39:PRO:HD3 | 2.40 | 0.41 |
| 27:G:34:ARG:HG2 | 27:G:34:ARG:NH1 | 2.35 | 0.41 |
| 20:J:43:GLU:O | 20:J:45:THR:HG22 | 2.20 | 0.41 |
| 2:B:28:A:O2' | 2:B:29:U:H5' | 2.21 | 0.41 |
| 29:T:38:ALA:HB1 | 29:T:43:ILE:HD11 | 2.02 | 0.41 |
| 2:B:2305:U:C1' | 26:F:132:ARG:HA | 2.50 | 0.41 |
| 10:O:27:LEU:H | 10:O:27:LEU:HD12 | 1.85 | 0.41 |
| 25:U:73:ASN:HD22 | 25:U:73:ASN:H | 1.69 | 0.41 |
| 26:F:41:GLU:CB | 26:F:48:LEU:HD11 | 2.51 | 0.41 |
| 12:1:36:LYS:NZ | 12:1:47:ILE:HG13 | 2.34 | 0.41 |
| 2:B:1031:G:N3 | 11:4:38:GLY:O | 2.53 | 0.41 |
| 2:B:847:U:H2' | 2:B:848:C:H6 | 1.85 | 0.41 |
| 2:B:231:A:H3' | 2:B:232:G:C8 | 2.55 | 0.41 |
| 2:B:1410:G:O2' | 2:B:1411:U:H5' | 2.21 | 0.41 |
| 2:B:1117:C:H2' | 2:B:1118:C:H6 | 1.85 | 0.41 |
| 2:B:2185:U:H2' | 2:B:2186:G:H8 | 1.86 | 0.41 |
| 21:N:12:ARG:HG3 | 21:N:13:ASN:N | 2.36 | 0.41 |
| 2:B:340:A:H2' | 2:B:341:C:C5' | 2.51 | 0.41 |
| 30:Z:40:VAL:HG21 | 30:Z:43:GLU:HB3 | 2.03 | 0.41 |
| 2:B:2320:U:O2' | 2:B:2322:A:N7 | 2.48 | 0.41 |
| 2:B:2457:U:C2' | 2:B:2458:G:H5' | 2.50 | 0.41 |
| 2:B:2405:G:H1' | 2:B:2412:A:N6 | 2.36 | 0.41 |
| 2:B:2836:U:H2' | 2:B:2837:A:H8 | 1.85 | 0.41 |
| 6:K:58:LEU:HB2 | 6:K:59:LYS:H | 1.63 | 0.41 |
| 2:B:1686:C:H2' | 2:B:1687:G:O4' | 2.20 | 0.41 |
| 2:B:1688:U:H2' | 2:B:1698:A:N6 | 2.36 | 0.41 |
| 2:B:1758:U:O4 | 2:B:2695:U:H4' | 2.21 | 0.41 |
| 2:B:257:C:H2' | 2:B:258:G:O4' | 2.21 | 0.41 |
| 25:U:2:ALA:O | 25:U:5:ARG:NH2 | 2.51 | 0.41 |
| 5:D:16:THR:HB | 5:D:18:ASP:OD1 | 2.20 | 0.41 |
| 2:B:2368:C:O2' | 2:B:2369:A:H5' | 2.21 | 0.41 |
| 31:W:48:ALA:HB3 | 31:W:81:ILE:O | 2.21 | 0.41 |
| 5:D:106:LYS:HG3 | 5:D:206:ALA:HB3 | 2.02 | 0.41 |
| 16:L:85:VAL:HG22 | 16:L:94:THR:CG2 | 2.50 | 0.41 |
| 27:G:8:VAL:HG12 | 27:G:9:VAL:N | 2.35 | 0.41 |
| 19:H:3:VAL:HA | 19:H:39:ALA:HB2 | 2.03 | 0.41 |
| 4:C:184:GLU:O | 4:C:185:ALA:HB3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 26:F:74:ALA:C | 26:F:76:PHE:N | 2.74 | 0.41 |
| 26:F:77:LYS:HG3 | 26:F:78:ILE:N | 2.35 | 0.41 |
| 2:B:443:A:H2 | 2:B:1245:G:N3 | 2.19 | 0.41 |
| 21:N:61:ALA:C | 21:N:63:ARG:H | 2.22 | 0.41 |
| 24:S:31:GLN:C | 24:S:33:LEU:N | 2.74 | 0.41 |
| 17:M:72:PRO:O | 17:M:91:TYR:O | 2.38 | 0.41 |
| 17:M:46:ILE:HG13 | 17:M:47:GLU:N | 2.36 | 0.41 |
| 26:F:33:ILE:HD13 | 26:F:98:PHE:CD2 | 2.41 | 0.41 |
| 24:S:47:VAL:HG12 | 24:S:103:ILE:HD13 | 2.03 | 0.41 |
| 2:B:543:G:N2 | 2:B:545:U:C5' | 2.83 | 0.41 |
| 6:K:47:ILE:HG23 | 6:K:48:PRO:N | 2.36 | 0.41 |
| 30:Z:54:LYS:HA | 30:Z:57:ARG:CD | 2.41 | 0.41 |
| 2:B:2531:A:H5' | 27:G:173:ALA:HB1 | 2.03 | 0.41 |
| 2:B:675:A:N3 | 2:B:2443:C:O2' | 2.48 | 0.41 |
| 15:2:21:ARG:C | 15:2:23:ALA:H | 2.24 | 0.41 |
| 2:B:1338:G:H4' | 29:T:18:GLU:CG | 2.44 | 0.41 |
| 2:B:928:A:H2 | 9:Y:46:MET:HE3 | 1.86 | 0.41 |
| 22:O:82:ALA:HB1 | 22:O:87:ILE:HB | 2.02 | 0.41 |
| 2:B:637:A:H4' | 2:B:638:G:O5' | 2.20 | 0.41 |
| 19:H:72:ILE:HD13 | 19:H:110:VAL:HB | 2.02 | 0.41 |
| 4:C:77:VAL:HA | 4:C:93:VAL:HA | 2.02 | 0.41 |
| 27:G:162:ARG:HG3 | 27:G:166:GLU:HG3 | 2.02 | 0.41 |
| 25:U:93:ARG:HB2 | 25:U:102:ILE:HG21 | 2.03 | 0.41 |
| 2:B:2798:U:H1' | 2:B:2800:A:H61 | 1.85 | 0.41 |
| 5:D:73:VAL:O | 5:D:74:GLU:HB2 | 2.20 | 0.41 |
| 7:P:61:ARG:HD3 | 7:P:70:GLU:HG3 | 2.03 | 0.41 |
| 31:W:41:GLY:HA2 | 31:W:44:PHE:CD2 | 2.55 | 0.41 |
| 4:C:254:LYS:O | 4:C:255:LYS:HD2 | 2.20 | 0.41 |
| 11:4:36:ARG:HG2 | 11:4:37:GLN:N | 2.36 | 0.41 |
| 2:B:65:U:H2' | 2:B:66:C:C6 | 2.53 | 0.41 |
| 30:Z:29:PHE:N | 30:Z:29:PHE:CD1 | 2.89 | 0.41 |
| 28:R:68:ARG:HD3 | 28:R:92:TRP:CE2 | 2.56 | 0.41 |
| 28:R:68:ARG:NH2 | 28:R:90:ARG:HB2 | 2.36 | 0.41 |
| 2:B:2882:A:OP1 | 21:N:96:ARG:HD2 | 2.21 | 0.41 |
| 25:U:41:VAL:O | 25:U:59:GLU:HG3 | 2.21 | 0.41 |
| 2:B:2793:C:H2' | 2:B:2794:C:H6 | 1.86 | 0.41 |
| 4:C:262:THR:C | 4:C:264:LYS:H | 2.25 | 0.41 |
| 2:B:329:G:O4' | 2:B:477:A:H1' | 2.21 | 0.41 |
| 5:D:124:ARG:HG3 | 5:D:125:TRP:CD1 | 2.56 | 0.41 |
| 2:B:2294:G:P | 22:O:94:ARG:NH1 | 2.92 | 0.41 |
| 2:B:1613:G:O4' | 15:2:3:ARG:HG3 | 2.21 | 0.41 |
| 2:B:2152:G:H2' | 2:B:2153:C:O4' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:C:31:PRO:O | 4:C:32:LEU:HD23 | 2.21 | 0.41 |
| 2:B:322:A:H1' | 2:B:339:U:O2 | 2.21 | 0.41 |
| 2:B:709:U:H2' | 2:B:710:U:H6 | 1.86 | 0.41 |
| 2:B:1948:G:C6 | 2:B:1959:G:C6 | 3.09 | 0.41 |
| 18:X:20:ASN:ND2 | 18:X:20:ASN:N | 2.69 | 0.41 |
| 19:H:67:ALA:O | 19:H:71:LYS:HG3 | 2.21 | 0.41 |
| 2:B:1461:C:H2' | 2:B:1462:C:H6 | 1.86 | 0.41 |
| 5:D:110:THR:HG23 | 5:D:171:THR:CB | 2.50 | 0.41 |
| 2:B:866:A:H61 | 2:B:913:U:C4' | 2.34 | 0.41 |
| 2:B:1858:A:H2' | 2:B:1859:U:O4' | 2.20 | 0.41 |
| 25:U:48:VAL:O | 25:U:48:VAL:HG22 | 2.20 | 0.41 |
| 2:B:93:G:H2' | 2:B:94:A:C8 | 2.56 | 0.41 |
| 29:T:6:ARG:HB3 | 29:T:6:ARG:CZ | 2.51 | 0.41 |
| 4:C:17:LYS:H | 4:C:17:LYS:HG3 | 1.64 | 0.41 |
| 13:3:26:ALA:O | 13:3:27:ASN:C | 2.59 | 0.41 |
| 2:B:2838:G:H2' | 2:B:2839:G:H8 | 1.86 | 0.41 |
| 2:B:2207:C:H2' | 2:B:2208:C:C6 | 2.55 | 0.41 |
| 2:B:1263:U:O2' | 10:0:7:PRO:HD2 | 2.20 | 0.41 |
| 21:N:69:ARG:HD3 | 21:N:69:ARG:H | 1.85 | 0.41 |
| 2:B:2236:U:O2' | 2:B:2237:G:H5' | 2.21 | 0.41 |
| 2:B:1361:G:H2' | 2:B:1362:C:C6 | 2.56 | 0.41 |
| 2:B:1099:G:C5' | 3:I:4:VAL:HG12 | 2.51 | 0.41 |
| 2:B:858:G:N2 | 2:B:2269:G:OP2 | 2.54 | 0.41 |
| 16:L:85:VAL:O | 16:L:86:GLU:HB3 | 2.21 | 0.41 |
| 27:G:31:GLU:O | 27:G:32:LEU:HB2 | 2.21 | 0.41 |
| 7:P:62:LYS:O | 7:P:63:ILE:HB | 2.21 | 0.41 |
| 5:D:25:THR:HG21 | 5:D:193:VAL:HG21 | 2.03 | 0.41 |
| 4:C:109:LEU:H | 4:C:109:LEU:CD2 | 2.34 | 0.41 |
| 30:Z:68:LEU:HD13 | 30:Z:78:TYR:CE1 | 2.55 | 0.41 |
| 12:1:49:LYS:HG3 | 12:1:50:GLU:N | 2.24 | 0.41 |
| 25:U:73:ASN:HD22 | 25:U:74:ALA:N | 2.19 | 0.41 |
| 19:H:126:GLY:H | 19:H:146:VAL:HB | 1.85 | 0.41 |
| 12:1:8:ILE:CD1 | 12:1:51:ALA:HA | 2.51 | 0.41 |
| 9:Y:58:GLU:CD | 9:Y:58:GLU:H | 2.23 | 0.41 |
| 25:U:72:PHE:CZ | 25:U:77:GLY:HA2 | 2.56 | 0.41 |
| 8:E:187:VAL:HG12 | 8:E:188:MET:N | 2.36 | 0.41 |
| 2:B:1882:U:O2' | 2:B:1883:U:H5' | 2.21 | 0.41 |
| 2:B:460:A:H4' | 29:T:72:GLN:HB3 | 2.03 | 0.41 |
| 13:3:7:ARG:HG3 | 13:3:7:ARG:NH1 | 2.36 | 0.41 |
| 2:B:590:A:H2' | 2:B:591:U:H6 | 1.86 | 0.41 |
| 4:C:181:ARG:NH2 | 4:C:181:ARG:HG2 | 2.35 | 0.41 |
| 2:B:1449:G:O2' | 2:B:1450:G:H5' | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:942:G:O2' | 2:B:943:A:H5' | 2.21 | 0.41 |
| 2:B:121:G:H4' | 2:B:149:A:H5' | 2.03 | 0.41 |
| 31:W:54:ARG:HG3 | 31:W:54:ARG:H | 1.60 | 0.41 |
| 2:B:1759:A:H4' | 2:B:2715:C:O4' | 2.21 | 0.41 |
| 2:B:755:U:H2' | 2:B:756:A:C8 | 2.55 | 0.41 |
| 2:B:1704:C:O2' | 2:B:1705:A:H5' | 2.21 | 0.41 |
| 31:W:59:PHE:CE2 | 31:W:61:LYS:HD2 | 2.55 | 0.40 |
| 16:L:101:ILE:HG22 | 16:L:102:GLY:N | 2.36 | 0.40 |
| 19:H:3:VAL:HA | 19:H:39:ALA:N | 2.36 | 0.40 |
| 14:V:93:ARG:HG3 | 14:V:93:ARG:H | 1.61 | 0.40 |
| 2:B:705:A:N6 | 2:B:726:G:O2' | 2.54 | 0.40 |
| 26:F:107:VAL:HB | 26:F:108:PRO:HD3 | 2.03 | 0.40 |
| 26:F:34:THR:OG1 | 26:F:154:THR:HB | 2.21 | 0.40 |
| 2:B:565:C:H2' | 2:B:566:U:O4' | 2.20 | 0.40 |
| 2:B:1439:A:C8 | 2:B:1440:U:C6 | 3.09 | 0.40 |
| 2:B:1443:U:H2' | 2:B:1444:G:H8 | 1.86 | 0.40 |
| 2:B:362:A:H2' | 2:B:363:G:H8 | 1.85 | 0.40 |
| 19:H:125:THR:CA | 19:H:146:VAL:HB | 2.46 | 0.40 |
| 6:K:73:ASP:OD2 | 6:K:75:SER:HB3 | 2.22 | 0.40 |
| 17:M:64:TRP:O | 17:M:103:TYR:HA | 2.21 | 0.40 |
| 8:E:47:LYS:CB | 8:E:51:GLU:HB2 | 2.44 | 0.40 |
| 2:B:2419:U:H2' | 2:B:2420:C:C6 | 2.56 | 0.40 |
| 2:B:532:A:HO2' | 2:B:2021:C:H5 | 1.63 | 0.40 |
| 18:X:53:VAL:O | 18:X:56:LEU:HB2 | 2.21 | 0.40 |
| 2:B:2425:A:H4' | 2:B:2426:A:OP2 | 2.21 | 0.40 |
| 1:A:103:U:O2' | 1:A:104:A:H5' | 2.20 | 0.40 |
| 25:U:40:LEU:HD23 | 25:U:59:GLU:HG2 | 2.03 | 0.40 |
| 2:B:2295:C:O2' | 2:B:2296:U:H5' | 2.20 | 0.40 |
| 8:E:34:ALA:CB | 8:E:96:VAL:HG21 | 2.50 | 0.40 |
| 2:B:2345:G:H4' | 2:B:2346:A:O5' | 2.21 | 0.40 |
| 2:B:2209:G:H2' | 2:B:2210:U:C5 | 2.56 | 0.40 |
| 14:V:2:PHE:HD2 | 14:V:59:GLU:OE1 | 2.04 | 0.40 |
| 2:B:622:G:H2' | 2:B:623:C:C6 | 2.56 | 0.40 |
| 2:B:353:C:N4 | 2:B:354:A:N6 | 2.69 | 0.40 |
| 2:B:2260:C:O2' | 2:B:2261:C:H5' | 2.21 | 0.40 |
| 6:K:59:LYS:HD2 | 6:K:89:ASN:HA | 2.03 | 0.40 |
| 2:B:68:G:H2' | 2:B:69:C:H6 | 1.85 | 0.40 |
| 2:B:2651:C:H2' | 2:B:2652:C:C6 | 2.56 | 0.40 |
| 2:B:1357:C:O2' | 2:B:1358:G:H5' | 2.21 | 0.40 |
| 3:I:56:VAL:CG2 | 3:I:68:PHE:HB2 | 2.51 | 0.40 |
| 16:L:14:LYS:O | 16:L:15:ALA:C | 2.59 | 0.40 |
| 2:B:2579:C:O5' | 2:B:2579:C:H6 | 2.05 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 7:P:6:GLN:C | 7:P:8:GLU:N | 2.74 | 0.40 |
| 4:C:89:ASN:O | 4:C:104:LEU:O | 2.39 | 0.40 |
| 3:I:108:ILE:CG2 | 3:I:128:ILE:HD13 | 2.51 | 0.40 |
| 9:Y:37:ARG:HG2 | 9:Y:43:ILE:CD1 | 2.51 | 0.40 |
| 22:O:39:VAL:HG12 | 22:O:48:LEU:HD12 | 2.03 | 0.40 |
| 19:H:113:SER:HB2 | 19:H:132:PHE:CZ | 2.56 | 0.40 |
| 7:P:59:THR:HA | 7:P:71:ARG:O | 2.20 | 0.40 |
| 3:I:105:LEU:HD11 | 3:I:139:VAL:CG2 | 2.45 | 0.40 |
| 6:K:78:ARG:HG3 | 6:K:78:ARG:HH11 | 1.86 | 0.40 |
| 2:B:1719:G:O2' | 2:B:1720:U:H5' | 2.21 | 0.40 |
| 7:P:45:VAL:H | 7:P:60:VAL:HB | 1.86 | 0.40 |
| 25:U:8:ASP:O | 25:U:23:LYS:HA | 2.21 | 0.40 |
| 22:O:51:ALA:HB3 | 22:O:78:VAL:HG22 | 2.03 | 0.40 |
| 2:B:1275:A:C4 | 21:N:16:HIS:CD2 | 3.08 | 0.40 |
| 1:A:91:C:H2' | 1:A:92:C:C6 | 2.56 | 0.40 |
| 2:B:2210:U:C4 | 2:B:2212:A:N6 | 2.89 | 0.40 |
| 2:B:2751:G:N3 | 2:B:2751:G:H2' | 2.36 | 0.40 |
| 3:I:63:ASP:OD1 | 3:I:63:ASP:O | 2.39 | 0.40 |
| 2:B:517:C:OP2 | 10:O:9:ARG:NH2 | 2.55 | 0.40 |
| 17:M:82:MET:O | 17:M:83:GLY:C | 2.60 | 0.40 |
| 2:B:2247:A:O2' | 2:B:2248:C:H5' | 2.21 | 0.40 |
| 6:K:89:ASN:HD22 | 6:K:89:ASN:C | 2.25 | 0.40 |
| 3:I:10:LEU:C | 3:I:10:LEU:HD12 | 2.41 | 0.40 |
| 20:J:134:ALA:HB3 | 20:J:135:GLN:HE22 | 1.86 | 0.40 |
| 35:B:4115:HOH:O | 20:J:39:LYS:HE3 | 2.22 | 0.40 |
| 27:G:150:TYR:O | 27:G:151:ARG:HD2 | 2.22 | 0.40 |
| 2:B:1237:A:HO2' | 2:B:1238:G:C4' | 2.34 | 0.40 |
| 2:B:1891:G:H2' | 2:B:1892:C:C6 | 2.57 | 0.40 |
| 3:I:14:ALA:HB3 | 3:I:51:GLY:H | 1.86 | 0.40 |
| 31:W:19:ARG:HE | 31:W:19:ARG:HB2 | 1.65 | 0.40 |
| 16:L:77:ILE:O | 16:L:110:VAL:O | 2.40 | 0.40 |
| 18:X:39:GLN:HB2 | 18:X:42:LEU:HB2 | 2.03 | 0.40 |
| 29:T:53:VAL:CG1 | 29:T:87:LEU:HD22 | 2.52 | 0.40 |
| 26:F:126:ASN:HD22 | 26:F:156:THR:HG23 | 1.86 | 0.40 |
| 24:S:6:LYS:CB | 24:S:104:THR:HA | 2.51 | 0.40 |
| 2:B:546:U:H4' | 2:B:548:G:OP2 | 2.22 | 0.40 |
| 20:J:18:VAL:HG13 | 20:J:56:VAL:HA | 2.03 | 0.40 |
| 19:H:5:LEU:HD13 | 19:H:14:SER:N | 2.36 | 0.40 |
| 2:B:2572:A:OP2 | 5:D:151:THR:HB | 2.21 | 0.40 |
| 2:B:783:A:H8 | 2:B:784:G:H4' | 1.85 | 0.40 |
| 2:B:1142:A:C4 | 2:B:1144:A:C8 | 3.10 | 0.40 |
| 10:O:37:HIS:CG | 10:O:43:THR:HG22 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 17:M:108:VAL:HG11 | 17:M:112:LEU:HD12 | 2.03 | 0.40 |
| 2:B:382:A:H2' | 2:B:383:C:O4' | 2.21 | 0.40 |
| 4:C:233:GLY:N | 4:C:241:LYS:HZ1 | 2.15 | 0.40 |
| 2:B:2492:U:C2' | 2:B:2493:U:H5' | 2.51 | 0.40 |
| 22:O:75:GLY:O | 22:O:110:ALA:HB2 | 2.22 | 0.40 |
| 2:B:1923:U:H2' | 2:B:1924:C:H6 | 1.86 | 0.40 |
| 2:B:2607:G:H2' | 2:B:2608:G:O4' | 2.21 | 0.40 |
| 2:B:1250:G:OP2 | 16:L:21:ARG:NH2 | 2.55 | 0.40 |
| 22:O:106:LEU:HG | 22:O:107:ALA:N | 2.34 | 0.40 |
| 2:B:1037:G:O2' | 2:B:1038:G:H5' | 2.21 | 0.40 |
| 2:B:1111:A:H3' | 2:B:1111:A:OP2 | 2.20 | 0.40 |
| 6:K:88:ASN:HD22 | 6:K:89:ASN:N | 2.20 | 0.40 |
| 6:K:39:ILE:HD13 | 6:K:39:ILE:H | 1.86 | 0.40 |
| 2:B:2076:U:O2 | 2:B:2076:U:O4' | 2.38 | 0.40 |
| 17:M:58:LYS:HD2 | 17:M:58:LYS:N | 2.36 | 0.40 |
| 2:B:955:U:H5' | 17:M:86:LYS:HE2 | 2.03 | 0.40 |
| 2:B:779:U:OP1 | 4:C:48:ILE:HG13 | 2.21 | 0.40 |
| 2:B:2586:U:H2' | 2:B:2587:A:C8 | 2.55 | 0.40 |
| 2:B:1370:C:H2' | 2:B:1371:G:O4' | 2.21 | 0.40 |
| 2:B:1098:A:C8 | 3:I:3:LYS:CB | 3.04 | 0.40 |
| 2:B:857:G:O2' | 31:W:19:ARG:HD2 | 2.21 | 0.40 |
| 31:W:23:LYS:O | 31:W:66:VAL:HB | 2.22 | 0.40 |
| 27:G:17:LYS:HG3 | 27:G:18:ILE:H | 1.86 | 0.40 |
| 5:D:60:VAL:HA | 5:D:64:GLU:OE2 | 2.21 | 0.40 |
| 29:T:29:THR:CB | 29:T:86:THR:HG22 | 2.50 | 0.40 |
| 4:C:90:ILE:HA | 4:C:90:ILE:HD13 | 1.85 | 0.40 |
| 11:4:2:LYS:HD3 | 11:4:4:ARG:NE | 2.30 | 0.40 |
| 8:E:29:HIS:O | 8:E:32:VAL:HG22 | 2.21 | 0.40 |
| 8:E:92:HIS:N | 8:E:92:HIS:ND1 | 2.70 | 0.40 |
| 19:H:5:LEU:CD1 | 19:H:13:GLY:HA2 | 2.51 | 0.40 |
| 20:J:80:HIS:O | 20:J:82:GLY:N | 2.54 | 0.40 |
| 19:H:133:GLN:CA | 19:H:139:PHE:HB3 | 2.49 | 0.40 |
| 8:E:146:VAL:HG12 | 8:E:147:LEU:N | 2.37 | 0.40 |
| 10:0:41:HIS:HB2 | 21:N:99:LYS:C | 2.40 | 0.40 |
| 2:B:2800:A:C2' | 2:B:2801:G:O4' | 2.63 | 0.40 |
| 26:F:134:GLN:HE21 | 26:F:134:GLN:HB3 | 1.62 | 0.40 |
| 2:B:63:A:OP2 | 2:B:63:A:H8 | 2.04 | 0.40 |
| 2:B:1228:G:O2' | 2:B:1229:C:H5' | 2.20 | 0.40 |
| 2:B:2883:A:OP1 | 10:0:48:TYR:CE1 | 2.75 | 0.40 |
| 2:B:2461:A:H1' | 2:B:2492:U:C2 | 2.56 | 0.40 |
| 2:B:2108:A:N3 | 2:B:2108:A:C2' | 2.84 | 0.40 |
| 2:B:674:G:H1' | 8:E:69:ARG:HE | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 2:B:175:G:O2' | 2:B:176:A:H5' | 2.22 | 0.40 |
| 2:B:1983:G:H4' | 2:B:2606:C:H4' | 2.04 | 0.40 |
| 2:B:2515:C:O2' | 2:B:2516:A:H5' | 2.22 | 0.40 |
| 2:B:1859:U:H2' | 2:B:1860:G:C8 | 2.56 | 0.40 |
| 2:B:1715:G:HO2' | 2:B:1743:G:H1 | 1.68 | 0.40 |
| 2:B:1774:C:H4' | 2:B:1979:U:O2 | 2.21 | 0.40 |
| 2:B:1064:C:O2' | 2:B:1065:U:H5' | 2.20 | 0.40 |
| 1:A:20:G:H2' | 1:A:21:G:C8 | 2.56 | 0.40 |
| 25:U:43:LYS:HD3 | 25:U:44:HIS:N | 2.37 | 0.40 |
| 26:F:140:ILE:HG13 | 26:F:140:ILE:H | 1.73 | 0.40 |
| 2:B:1696:G:H8 | 2:B:1696:G:OP2 | 2.04 | 0.40 |
| 2:B:1678:A:H2' | 2:B:1679:A:O4' | 2.21 | 0.40 |
| 2:B:1985:C:O2' | 2:B:1986:C:H5' | 2.22 | 0.40 |
| 2:B:1533:C:O2' | 2:B:1534:U:H5' | 2.22 | 0.40 |
| 2:B:1456:G:O2' | 2:B:1457:U:H5' | 2.22 | 0.40 |
| 2:B:736:C:H2' | 2:B:737:C:C6 | 2.57 | 0.40 |
| 2:B:917:A:H5'' | 2:B:2268:A:N6 | 2.35 | 0.40 |
| 5:D:107:VAL:O | 5:D:174:SER:O | 2.39 | 0.40 |
| 16:L:141:LYS:NZ | 16:L:143:GLU:HA | 2.36 | 0.40 |
| 8:E:155:GLU:O | 8:E:159:LEU:HD13 | 2.21 | 0.40 |
| 27:G:33:THR:HA | 27:G:34:ARG:NH1 | 2.37 | 0.40 |
| 23:Q:91:ARG:HD3 | 28:R:11:GLN:CG | 2.51 | 0.40 |
| 2:B:1176:U:C6 | 2:B:1176:U:P | 3.14 | 0.40 |
| 2:B:2874:C:H2' | 2:B:2875:C:C6 | 2.57 | 0.40 |
| 7:P:6:GLN:O | 7:P:10:GLU:HB3 | 2.21 | 0.40 |
| 2:B:1438:U:C4 | 2:B:1552:A:N6 | 2.90 | 0.40 |
| 8:E:145:ASP:CA | 8:E:166:LYS:HB3 | 2.41 | 0.40 |
| 9:Y:37:ARG:HG2 | 9:Y:43:ILE:HD11 | 2.03 | 0.40 |
| 2:B:2732:G:N3 | 2:B:2732:G:O4' | 2.55 | 0.40 |
| 16:L:115:GLU:OE1 | 16:L:115:GLU:N | 2.54 | 0.40 |
| 25:U:93:ARG:HB2 | 25:U:102:ILE:CG2 | 2.51 | 0.40 |
| 25:U:73:ASN:ND2 | 25:U:74:ALA:N | 2.70 | 0.40 |
| 2:B:533:G:H5' | 23:Q:23:TYR:CD2 | 2.57 | 0.40 |
| 15:2:18:PHE:CE1 | 15:2:22:MET:HG3 | 2.57 | 0.40 |
| 2:B:1708:C:O2' | 2:B:1709:U:H5' | 2.21 | 0.40 |
| 2:B:1693:U:H4' | 2:B:1694:C:OP2 | 2.21 | 0.40 |
| 8:E:191:ASP:O | 8:E:194:LYS:HB3 | 2.20 | 0.40 |
| 27:G:10:VAL:HG11 | 27:G:16:VAL:HG21 | 2.04 | 0.40 |
| 2:B:876:C:H2' | 2:B:877:A:C1' | 2.52 | 0.40 |
| 2:B:878:A:H5' | 2:B:900:A:N1 | 2.37 | 0.40 |
| 2:B:1197:G:C4 | 2:B:1198:U:C5 | 3.09 | 0.40 |
| 2:B:303:G:H2' | 2:B:304:U:H6 | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:B:1921:G:O2' | 2:B:1922:G:H5' | 2.21 | 0.40 |
| 2:B:2347:C:OP1 | 2:B:2347:C:H4' | 2.22 | 0.40 |
| 2:B:958:U:P | 17:M:14:LYS:HZ3 | 2.45 | 0.40 |
| 28:R:79:ARG:O | 28:R:81:LYS:N | 2.55 | 0.40 |
| 22:O:105:ALA:C | 22:O:107:ALA:N | 2.75 | 0.40 |
| 12:1:39:ASP:OD1 | 12:1:42:VAL:HG23 | 2.21 | 0.40 |
| 2:B:747:U:OP2 | 24:S:90:LYS:NZ | 2.54 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3 | I | 139/141 (99%) | 115 (83%) | 19 (14%) | 5 (4%) | 5 | 50 |
| 4 | C | 269/272 (99%) | 167 (62%) | 59 (22%) | 43 (16%) | 0 | 5 |
| 5 | D | 207/209 (99%) | 119 (58%) | 59 (28%) | 29 (14%) | 0 | 8 |
| 6 | K | 119/123 (97%) | 78 (66%) | 23 (19%) | 18 (15%) | 0 | 6 |
| 7 | P | 112/114 (98%) | 60 (54%) | 37 (33%) | 15 (13%) | 0 | 9 |
| 8 | E | 199/201 (99%) | 127 (64%) | 46 (23%) | 26 (13%) | 0 | 10 |
| 9 | Y | 56/58 (97%) | 40 (71%) | 13 (23%) | 3 (5%) | 3 | 36 |
| 10 | 0 | 54/56 (96%) | 42 (78%) | 7 (13%) | 5 (9%) | 1 | 18 |
| 11 | 4 | 36/38 (95%) | 18 (50%) | 7 (19%) | 11 (31%) | 0 | 0 |
| 12 | 1 | 48/54 (89%) | 33 (69%) | 10 (21%) | 5 (10%) | 1 | 15 |
| 13 | 3 | 62/64 (97%) | 41 (66%) | 16 (26%) | 5 (8%) | 1 | 22 |
| 14 | V | 92/94 (98%) | 67 (73%) | 21 (23%) | 4 (4%) | 4 | 43 |
| 15 | 2 | 44/46 (96%) | 37 (84%) | 4 (9%) | 3 (7%) | 2 | 28 |
| 16 | L | 141/144 (98%) | 90 (64%) | 27 (19%) | 24 (17%) | 0 | 4 |
| 17 | M | 134/136 (98%) | 81 (60%) | 39 (29%) | 14 (10%) | 1 | 15 |
| 18 | X | 61/63 (97%) | 37 (61%) | 17 (28%) | 7 (12%) | 1 | 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 19 | H | 147/149 (99%) | 89 (60%) | 30 (20%) | 28 (19%) | 0 | 3 |
| 20 | J | 140/142 (99%) | 85 (61%) | 36 (26%) | 19 (14%) | 0 | 8 |
| 21 | N | 118/127 (93%) | 76 (64%) | 30 (25%) | 12 (10%) | 1 | 15 |
| 22 | O | 114/117 (97%) | 80 (70%) | 23 (20%) | 11 (10%) | 1 | 17 |
| 23 | Q | 115/117 (98%) | 77 (67%) | 30 (26%) | 8 (7%) | 2 | 27 |
| 24 | S | 108/110 (98%) | 66 (61%) | 29 (27%) | 13 (12%) | 1 | 12 |
| 25 | U | 100/103 (97%) | 59 (59%) | 23 (23%) | 18 (18%) | 0 | 4 |
| 26 | F | 176/178 (99%) | 102 (58%) | 49 (28%) | 25 (14%) | 0 | 8 |
| 27 | G | 174/176 (99%) | 94 (54%) | 50 (29%) | 30 (17%) | 0 | 4 |
| 28 | R | 101/103 (98%) | 62 (61%) | 26 (26%) | 13 (13%) | 0 | 10 |
| 29 | T | 91/100 (91%) | 51 (56%) | 23 (25%) | 17 (19%) | 0 | 3 |
| 30 | Z | 75/78 (96%) | 50 (67%) | 15 (20%) | 10 (13%) | 0 | 9 |
| 31 | W | 77/84 (92%) | 30 (39%) | 24 (31%) | 23 (30%) | 0 | 0 |
| All | All | 3309/3397 (97%) | 2073 (63%) | 792 (24%) | 444 (13%) | 0 | 9 |

All (444) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 5 | GLN |
| 3 | I | 18 | ASN |
| 4 | C | 4 | LYS |
| 4 | C | 53 | ILE |
| 4 | C | 77 | VAL |
| 4 | C | 135 | PRO |
| 4 | C | 141 | HIS |
| 5 | D | 9 | VAL |
| 5 | D | 74 | GLU |
| 5 | D | 91 | THR |
| 5 | D | 107 | VAL |
| 5 | D | 112 | THR |
| 5 | D | 122 | VAL |
| 5 | D | 169 | ARG |
| 5 | D | 184 | ARG |
| 5 | D | 194 | PRO |
| 6 | K | 31 | ARG |
| 6 | K | 35 | VAL |
| 6 | K | 72 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | K | 119 | ALA |
| 6 | K | 120 | PRO |
| 7 | P | 25 | VAL |
| 7 | P | 50 | ARG |
| 7 | P | 64 | SER |
| 7 | P | 75 | THR |
| 8 | E | 45 | ALA |
| 8 | E | 61 | ARG |
| 8 | E | 62 | GLN |
| 8 | E | 79 | ARG |
| 8 | E | 165 | HIS |
| 8 | E | 167 | VAL |
| 10 | O | 23 | ALA |
| 10 | O | 42 | ILE |
| 10 | O | 51 | ARG |
| 13 | 3 | 31 | ILE |
| 16 | L | 66 | PHE |
| 16 | L | 89 | VAL |
| 16 | L | 100 | ILE |
| 16 | L | 111 | ILE |
| 16 | L | 116 | VAL |
| 17 | M | 78 | LEU |
| 18 | X | 2 | LYS |
| 19 | H | 10 | ALA |
| 19 | H | 14 | SER |
| 19 | H | 31 | VAL |
| 19 | H | 32 | PRO |
| 19 | H | 33 | GLN |
| 19 | H | 89 | LYS |
| 19 | H | 93 | SER |
| 20 | J | 4 | PHE |
| 20 | J | 44 | TYR |
| 20 | J | 45 | THR |
| 20 | J | 52 | ASP |
| 20 | J | 73 | VAL |
| 20 | J | 81 | ILE |
| 20 | J | 111 | LYS |
| 20 | J | 124 | VAL |
| 21 | N | 11 | ASN |
| 21 | N | 82 | GLU |
| 24 | S | 3 | THR |
| 24 | S | 13 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | U | 6 | ARG |
| 25 | U | 18 | LYS |
| 25 | U | 49 | PRO |
| 25 | U | 50 | ALA |
| 26 | F | 32 | LYS |
| 26 | F | 87 | LYS |
| 26 | F | 110 | ILE |
| 26 | F | 112 | ASP |
| 26 | F | 138 | PRO |
| 26 | F | 149 | ARG |
| 27 | G | 7 | PRO |
| 27 | G | 8 | VAL |
| 27 | G | 11 | PRO |
| 27 | G | 85 | LYS |
| 27 | G | 91 | VAL |
| 27 | G | 94 | ARG |
| 27 | G | 117 | PRO |
| 28 | R | 7 | SER |
| 29 | T | 16 | VAL |
| 29 | T | 39 | THR |
| 29 | T | 58 | VAL |
| 29 | T | 88 | LYS |
| 30 | Z | 33 | LEU |
| 30 | Z | 45 | ARG |
| 30 | Z | 46 | PHE |
| 30 | Z | 77 | LYS |
| 31 | W | 9 | THR |
| 31 | W | 14 | ASP |
| 31 | W | 30 | VAL |
| 31 | W | 50 | VAL |
| 31 | W | 70 | VAL |
| 4 | C | 17 | LYS |
| 4 | C | 34 | GLU |
| 4 | C | 35 | LYS |
| 4 | C | 36 | ASN |
| 4 | C | 37 | SER |
| 4 | C | 52 | HIS |
| 4 | C | 59 | GLN |
| 4 | C | 63 | ILE |
| 4 | C | 64 | VAL |
| 4 | C | 93 | VAL |
| 4 | C | 94 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 140 | VAL |
| 4 | C | 142 | ASN |
| 4 | C | 145 | MET |
| 4 | C | 239 | PHE |
| 5 | D | 31 | ALA |
| 5 | D | 93 | GLY |
| 5 | D | 95 | SER |
| 5 | D | 102 | ALA |
| 5 | D | 106 | LYS |
| 5 | D | 121 | THR |
| 5 | D | 145 | SER |
| 5 | D | 170 | VAL |
| 5 | D | 182 | ALA |
| 6 | K | 16 | ALA |
| 6 | K | 17 | ARG |
| 6 | K | 73 | ASP |
| 6 | K | 80 | ASP |
| 6 | K | 92 | GLU |
| 6 | K | 101 | GLY |
| 6 | K | 110 | GLU |
| 7 | P | 31 | VAL |
| 7 | P | 37 | LYS |
| 8 | E | 42 | GLY |
| 8 | E | 69 | ARG |
| 8 | E | 150 | THR |
| 8 | E | 166 | LYS |
| 9 | Y | 4 | ILE |
| 11 | 4 | 7 | VAL |
| 11 | 4 | 8 | LYS |
| 11 | 4 | 9 | LYS |
| 11 | 4 | 23 | ILE |
| 11 | 4 | 34 | LYS |
| 12 | 1 | 4 | ILE |
| 13 | 3 | 50 | SER |
| 14 | V | 75 | GLN |
| 15 | 2 | 44 | VAL |
| 15 | 2 | 45 | SER |
| 16 | L | 51 | GLU |
| 16 | L | 143 | GLU |
| 17 | M | 13 | HIS |
| 17 | M | 19 | GLY |
| 17 | M | 56 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | M | 58 | LYS |
| 17 | M | 69 | PRO |
| 17 | M | 83 | GLY |
| 17 | M | 106 | ASP |
| 17 | M | 116 | ALA |
| 17 | M | 134 | THR |
| 18 | X | 9 | LYS |
| 18 | X | 58 | ASN |
| 19 | H | 3 | VAL |
| 19 | H | 6 | LEU |
| 19 | H | 8 | LYS |
| 19 | H | 11 | ASN |
| 19 | H | 86 | ASP |
| 19 | H | 91 | PHE |
| 19 | H | 107 | GLY |
| 19 | H | 148 | ALA |
| 20 | J | 2 | LYS |
| 20 | J | 43 | GLU |
| 20 | J | 83 | GLY |
| 21 | N | 10 | LEU |
| 21 | N | 101 | GLY |
| 22 | O | 68 | LYS |
| 23 | Q | 4 | LYS |
| 23 | Q | 10 | ARG |
| 23 | Q | 85 | ALA |
| 23 | Q | 86 | SER |
| 23 | Q | 87 | VAL |
| 24 | S | 14 | ALA |
| 24 | S | 40 | ASN |
| 24 | S | 63 | GLY |
| 24 | S | 65 | ASP |
| 24 | S | 96 | ILE |
| 25 | U | 16 | LYS |
| 25 | U | 61 | GLU |
| 25 | U | 85 | ARG |
| 25 | U | 92 | VAL |
| 26 | F | 9 | ASP |
| 26 | F | 11 | VAL |
| 26 | F | 78 | ILE |
| 26 | F | 92 | GLY |
| 26 | F | 135 | ILE |
| 26 | F | 148 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | G | 84 | LYS |
| 27 | G | 102 | ILE |
| 27 | G | 111 | PRO |
| 27 | G | 125 | PRO |
| 27 | G | 170 | THR |
| 27 | G | 174 | LYS |
| 28 | R | 70 | GLU |
| 29 | T | 10 | VAL |
| 29 | T | 11 | LEU |
| 29 | T | 19 | LYS |
| 29 | T | 38 | ALA |
| 30 | Z | 35 | SER |
| 30 | Z | 70 | GLU |
| 30 | Z | 71 | LEU |
| 31 | W | 32 | ALA |
| 31 | W | 58 | LEU |
| 31 | W | 61 | LYS |
| 3 | I | 23 | VAL |
| 4 | C | 3 | VAL |
| 4 | C | 65 | ASP |
| 4 | C | 202 | ARG |
| 4 | C | 203 | VAL |
| 4 | C | 237 | ARG |
| 4 | C | 250 | GLN |
| 4 | C | 254 | LYS |
| 5 | D | 136 | ASN |
| 5 | D | 159 | LYS |
| 5 | D | 164 | GLN |
| 6 | K | 6 | THR |
| 6 | K | 14 | SER |
| 6 | K | 46 | ALA |
| 6 | K | 90 | ASN |
| 7 | P | 30 | TRP |
| 7 | P | 38 | ARG |
| 7 | P | 65 | ASN |
| 7 | P | 86 | LYS |
| 8 | E | 46 | GLN |
| 8 | E | 70 | SER |
| 9 | Y | 2 | LYS |
| 9 | Y | 34 | THR |
| 10 | 0 | 54 | ILE |
| 11 | 4 | 4 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | 4 | 18 | LYS |
| 11 | 4 | 37 | GLN |
| 15 | 2 | 5 | PHE |
| 16 | L | 3 | LEU |
| 16 | L | 4 | ASN |
| 16 | L | 41 | ARG |
| 16 | L | 54 | GLN |
| 16 | L | 93 | ASN |
| 16 | L | 94 | THR |
| 17 | M | 20 | LEU |
| 17 | M | 72 | PRO |
| 18 | X | 36 | GLN |
| 19 | H | 9 | VAL |
| 19 | H | 12 | LEU |
| 19 | H | 56 | ALA |
| 19 | H | 92 | GLY |
| 19 | H | 96 | THR |
| 20 | J | 129 | GLU |
| 21 | N | 68 | ALA |
| 21 | N | 100 | CYS |
| 22 | O | 22 | GLY |
| 22 | O | 79 | ALA |
| 22 | O | 99 | TYR |
| 22 | O | 100 | HIS |
| 23 | Q | 88 | GLU |
| 25 | U | 59 | GLU |
| 26 | F | 41 | GLU |
| 26 | F | 175 | PRO |
| 27 | G | 2 | ARG |
| 27 | G | 45 | ALA |
| 27 | G | 89 | VAL |
| 27 | G | 157 | LYS |
| 28 | R | 24 | LYS |
| 28 | R | 40 | MET |
| 28 | R | 44 | GLY |
| 28 | R | 48 | LYS |
| 28 | R | 65 | ALA |
| 29 | T | 28 | ASN |
| 29 | T | 35 | ALA |
| 29 | T | 65 | GLY |
| 29 | T | 91 | GLN |
| 30 | Z | 3 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | W | 15 | SER |
| 31 | W | 34 | SER |
| 31 | W | 36 | ILE |
| 31 | W | 62 | ALA |
| 4 | C | 18 | VAL |
| 4 | C | 92 | LEU |
| 4 | C | 105 | ALA |
| 4 | C | 189 | ALA |
| 4 | C | 190 | THR |
| 4 | C | 196 | ASN |
| 4 | C | 222 | THR |
| 5 | D | 36 | GLN |
| 5 | D | 75 | ALA |
| 5 | D | 119 | ALA |
| 7 | P | 4 | ILE |
| 8 | E | 5 | LEU |
| 8 | E | 43 | THR |
| 8 | E | 73 | ILE |
| 8 | E | 162 | ARG |
| 8 | E | 188 | MET |
| 11 | 4 | 11 | CYS |
| 11 | 4 | 16 | ILE |
| 12 | 1 | 36 | LYS |
| 12 | 1 | 50 | GLU |
| 12 | 1 | 51 | ALA |
| 13 | 3 | 6 | VAL |
| 14 | V | 71 | LYS |
| 16 | L | 5 | THR |
| 16 | L | 28 | GLY |
| 16 | L | 29 | LYS |
| 16 | L | 36 | LYS |
| 16 | L | 81 | ASP |
| 17 | M | 77 | PRO |
| 18 | X | 45 | GLN |
| 19 | H | 5 | LEU |
| 19 | H | 7 | ASP |
| 19 | H | 15 | LEU |
| 19 | H | 29 | PHE |
| 19 | H | 113 | SER |
| 20 | J | 13 | ARG |
| 20 | J | 84 | ILE |
| 21 | N | 83 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | N | 98 | LEU |
| 22 | O | 13 | ARG |
| 22 | O | 57 | ALA |
| 22 | O | 98 | GLN |
| 23 | Q | 89 | ILE |
| 24 | S | 25 | ARG |
| 24 | S | 61 | ASN |
| 25 | U | 5 | ARG |
| 25 | U | 62 | ALA |
| 26 | F | 77 | LYS |
| 26 | F | 81 | GLY |
| 27 | G | 18 | ILE |
| 27 | G | 32 | LEU |
| 27 | G | 61 | TRP |
| 27 | G | 96 | ALA |
| 27 | G | 97 | VAL |
| 27 | G | 109 | SER |
| 28 | R | 80 | ARG |
| 28 | R | 91 | GLN |
| 29 | T | 86 | THR |
| 31 | W | 10 | ARG |
| 31 | W | 29 | SER |
| 31 | W | 40 | ARG |
| 31 | W | 60 | ALA |
| 31 | W | 76 | ARG |
| 31 | W | 78 | PHE |
| 3 | I | 6 | ALA |
| 3 | I | 14 | ALA |
| 4 | C | 88 | ALA |
| 4 | C | 121 | ALA |
| 4 | C | 123 | ILE |
| 4 | C | 131 | MET |
| 4 | C | 150 | GLY |
| 4 | C | 249 | VAL |
| 5 | D | 109 | VAL |
| 7 | P | 76 | HIS |
| 7 | P | 100 | ARG |
| 8 | E | 86 | ALA |
| 10 | 0 | 26 | SER |
| 13 | 3 | 58 | ILE |
| 16 | L | 9 | ALA |
| 16 | L | 19 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | L | 86 | GLU |
| 18 | X | 62 | GLY |
| 19 | H | 112 | LYS |
| 20 | J | 14 | ASP |
| 20 | J | 72 | LYS |
| 21 | N | 18 | GLN |
| 21 | N | 81 | ASN |
| 22 | O | 8 | ILE |
| 22 | O | 51 | ALA |
| 24 | S | 80 | PRO |
| 25 | U | 12 | VAL |
| 25 | U | 51 | LEU |
| 25 | U | 101 | THR |
| 26 | F | 35 | LEU |
| 26 | F | 93 | GLU |
| 26 | F | 103 | ILE |
| 26 | F | 158 | THR |
| 27 | G | 9 | VAL |
| 27 | G | 151 | ARG |
| 27 | G | 152 | ARG |
| 28 | R | 43 | ASN |
| 28 | R | 52 | PRO |
| 28 | R | 98 | ILE |
| 28 | R | 101 | ILE |
| 30 | Z | 34 | HIS |
| 31 | W | 27 | GLY |
| 31 | W | 37 | VAL |
| 5 | D | 172 | VAL |
| 6 | K | 3 | GLN |
| 8 | E | 59 | PRO |
| 8 | E | 78 | TRP |
| 8 | E | 83 | VAL |
| 8 | E | 96 | VAL |
| 8 | E | 123 | LYS |
| 14 | V | 84 | PRO |
| 16 | L | 15 | ALA |
| 17 | M | 73 | ILE |
| 19 | H | 119 | ASN |
| 20 | J | 112 | GLY |
| 21 | N | 60 | VAL |
| 21 | N | 104 | ALA |
| 24 | S | 18 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | U | 24 | VAL |
| 25 | U | 63 | ALA |
| 25 | U | 82 | VAL |
| 26 | F | 88 | VAL |
| 29 | T | 29 | THR |
| 29 | T | 55 | VAL |
| 29 | T | 83 | ALA |
| 31 | W | 51 | GLY |
| 31 | W | 73 | PRO |
| 4 | C | 151 | GLY |
| 6 | K | 93 | GLN |
| 8 | E | 129 | PRO |
| 11 | 4 | 17 | VAL |
| 14 | V | 37 | PRO |
| 22 | O | 27 | VAL |
| 26 | F | 28 | PRO |
| 26 | F | 123 | GLY |
| 26 | F | 136 | ILE |
| 27 | G | 112 | VAL |
| 27 | G | 155 | PRO |
| 7 | P | 17 | PRO |
| 18 | X | 46 | VAL |
| 20 | J | 8 | PRO |
| 20 | J | 54 | ILE |
| 24 | S | 24 | ILE |
| 27 | G | 16 | VAL |
| 27 | G | 168 | VAL |
| 4 | C | 31 | PRO |
| 4 | C | 158 | GLY |
| 5 | D | 143 | PRO |
| 8 | E | 187 | VAL |
| 12 | 1 | 30 | PRO |
| 13 | 3 | 20 | GLY |
| 16 | L | 101 | ILE |
| 19 | H | 121 | VAL |
| 23 | Q | 39 | ILE |
| 26 | F | 12 | VAL |
| 29 | T | 57 | VAL |
| 30 | Z | 47 | VAL |
| 31 | W | 53 | GLY |
| 16 | L | 52 | GLY |
| 25 | U | 41 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | D | 73 | VAL |
| 5 | D | 92 | VAL |
| 7 | P | 63 | ILE |
| 8 | E | 177 | PRO |
| 24 | S | 29 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | I | 109/109 (100%) | 103 (94%) | 6 (6%) | 30 | 78 |
| 4 | C | 216/217 (100%) | 183 (85%) | 33 (15%) | 4 | 25 |
| 5 | D | 164/164 (100%) | 138 (84%) | 26 (16%) | 4 | 22 |
| 6 | K | 102/104 (98%) | 77 (76%) | 25 (24%) | 1 | 6 |
| 7 | P | 99/99 (100%) | 81 (82%) | 18 (18%) | 2 | 15 |
| 8 | E | 165/165 (100%) | 144 (87%) | 21 (13%) | 6 | 34 |
| 9 | Y | 48/48 (100%) | 37 (77%) | 11 (23%) | 1 | 7 |
| 10 | 0 | 47/47 (100%) | 38 (81%) | 9 (19%) | 2 | 13 |
| 11 | 4 | 34/34 (100%) | 28 (82%) | 6 (18%) | 3 | 16 |
| 12 | 1 | 45/48 (94%) | 37 (82%) | 8 (18%) | 2 | 16 |
| 13 | 3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 12 | 50 |
| 14 | V | 78/78 (100%) | 63 (81%) | 15 (19%) | 2 | 12 |
| 15 | 2 | 38/38 (100%) | 31 (82%) | 7 (18%) | 2 | 14 |
| 16 | L | 102/103 (99%) | 91 (89%) | 11 (11%) | 9 | 44 |
| 17 | M | 109/109 (100%) | 93 (85%) | 16 (15%) | 4 | 27 |
| 18 | X | 55/55 (100%) | 49 (89%) | 6 (11%) | 9 | 44 |
| 19 | H | 114/114 (100%) | 91 (80%) | 23 (20%) | 2 | 11 |
| 20 | J | 116/116 (100%) | 98 (84%) | 18 (16%) | 4 | 24 |
| 21 | N | 100/103 (97%) | 86 (86%) | 14 (14%) | 5 | 29 |
| 22 | O | 86/87 (99%) | 68 (79%) | 18 (21%) | 1 | 10 |
| 23 | Q | 89/89 (100%) | 80 (90%) | 9 (10%) | 11 | 49 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 24 | S | 93/93 (100%) | 76 (82%) | 17 (18%) | 2 | 14 |
| 25 | U | 83/84 (99%) | 68 (82%) | 15 (18%) | 2 | 15 |
| 26 | F | 149/149 (100%) | 116 (78%) | 33 (22%) | 1 | 8 |
| 27 | G | 137/137 (100%) | 113 (82%) | 24 (18%) | 3 | 17 |
| 28 | R | 84/84 (100%) | 71 (84%) | 13 (16%) | 4 | 24 |
| 29 | T | 80/84 (95%) | 68 (85%) | 12 (15%) | 4 | 26 |
| 30 | Z | 67/68 (98%) | 54 (81%) | 13 (19%) | 2 | 12 |
| 31 | W | 59/62 (95%) | 44 (75%) | 15 (25%) | 1 | 6 |
| All | All | 2719/2739 (99%) | 2272 (84%) | 447 (16%) | 3 | 21 |

All (447) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 2 | LYS |
| 3 | I | 54 | ILE |
| 3 | I | 91 | LYS |
| 3 | I | 99 | LYS |
| 3 | I | 121 | ILE |
| 3 | I | 140 | GLU |
| 4 | C | 4 | LYS |
| 4 | C | 8 | THR |
| 4 | C | 12 | ARG |
| 4 | C | 43 | ASN |
| 4 | C | 44 | ASN |
| 4 | C | 45 | ASN |
| 4 | C | 52 | HIS |
| 4 | C | 62 | ARG |
| 4 | C | 65 | ASP |
| 4 | C | 89 | ASN |
| 4 | C | 90 | ILE |
| 4 | C | 100 | ARG |
| 4 | C | 123 | ILE |
| 4 | C | 134 | ILE |
| 4 | C | 142 | ASN |
| 4 | C | 155 | ARG |
| 4 | C | 166 | ARG |
| 4 | C | 172 | THR |
| 4 | C | 173 | LEU |
| 4 | C | 176 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 180 | MET |
| 4 | C | 190 | THR |
| 4 | C | 191 | LEU |
| 4 | C | 202 | ARG |
| 4 | C | 203 | VAL |
| 4 | C | 212 | TRP |
| 4 | C | 224 | MET |
| 4 | C | 235 | GLU |
| 4 | C | 249 | VAL |
| 4 | C | 257 | ARG |
| 4 | C | 264 | LYS |
| 4 | C | 267 | VAL |
| 4 | C | 268 | ARG |
| 5 | D | 17 | GLU |
| 5 | D | 24 | VAL |
| 5 | D | 34 | VAL |
| 5 | D | 35 | THR |
| 5 | D | 36 | GLN |
| 5 | D | 40 | LEU |
| 5 | D | 46 | ARG |
| 5 | D | 56 | LYS |
| 5 | D | 60 | VAL |
| 5 | D | 79 | LEU |
| 5 | D | 84 | LEU |
| 5 | D | 89 | GLU |
| 5 | D | 99 | GLU |
| 5 | D | 110 | THR |
| 5 | D | 116 | LYS |
| 5 | D | 123 | LYS |
| 5 | D | 124 | ARG |
| 5 | D | 129 | THR |
| 5 | D | 138 | LEU |
| 5 | D | 148 | GLN |
| 5 | D | 151 | THR |
| 5 | D | 154 | LYS |
| 5 | D | 159 | LYS |
| 5 | D | 179 | ARG |
| 5 | D | 185 | ASN |
| 5 | D | 204 | LYS |
| 6 | K | 2 | ILE |
| 6 | K | 8 | LEU |
| 6 | K | 21 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | K | 32 | TYR |
| 6 | K | 39 | ILE |
| 6 | K | 47 | ILE |
| 6 | K | 52 | VAL |
| 6 | K | 53 | LYS |
| 6 | K | 54 | LYS |
| 6 | K | 58 | LEU |
| 6 | K | 64 | ARG |
| 6 | K | 71 | ARG |
| 6 | K | 72 | PRO |
| 6 | K | 79 | PHE |
| 6 | K | 87 | LEU |
| 6 | K | 88 | ASN |
| 6 | K | 89 | ASN |
| 6 | K | 91 | SER |
| 6 | K | 98 | ARG |
| 6 | K | 104 | THR |
| 6 | K | 105 | ARG |
| 6 | K | 108 | ARG |
| 6 | K | 111 | LYS |
| 6 | K | 118 | LEU |
| 6 | K | 120 | PRO |
| 7 | P | 3 | ILE |
| 7 | P | 6 | GLN |
| 7 | P | 12 | MET |
| 7 | P | 19 | PHE |
| 7 | P | 20 | ARG |
| 7 | P | 25 | VAL |
| 7 | P | 26 | GLU |
| 7 | P | 33 | GLU |
| 7 | P | 37 | LYS |
| 7 | P | 38 | ARG |
| 7 | P | 43 | GLU |
| 7 | P | 61 | ARG |
| 7 | P | 83 | ILE |
| 7 | P | 99 | LEU |
| 7 | P | 100 | ARG |
| 7 | P | 101 | GLU |
| 7 | P | 111 | GLU |
| 7 | P | 112 | ARG |
| 8 | E | 9 | GLN |
| 8 | E | 22 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | E | 24 | ASN |
| 8 | E | 40 | ARG |
| 8 | E | 48 | THR |
| 8 | E | 58 | LYS |
| 8 | E | 60 | TRP |
| 8 | E | 67 | ARG |
| 8 | E | 78 | TRP |
| 8 | E | 108 | ILE |
| 8 | E | 111 | GLU |
| 8 | E | 115 | GLN |
| 8 | E | 116 | ASP |
| 8 | E | 118 | LEU |
| 8 | E | 122 | GLU |
| 8 | E | 124 | PHE |
| 8 | E | 147 | LEU |
| 8 | E | 163 | ASN |
| 8 | E | 170 | ARG |
| 8 | E | 191 | ASP |
| 8 | E | 198 | GLU |
| 9 | Y | 2 | LYS |
| 9 | Y | 6 | ILE |
| 9 | Y | 15 | ARG |
| 9 | Y | 16 | LEU |
| 9 | Y | 19 | HIS |
| 9 | Y | 23 | LEU |
| 9 | Y | 30 | ARG |
| 9 | Y | 37 | ARG |
| 9 | Y | 40 | THR |
| 9 | Y | 46 | MET |
| 9 | Y | 57 | GLU |
| 10 | 0 | 5 | ASN |
| 10 | 0 | 27 | LEU |
| 10 | 0 | 37 | HIS |
| 10 | 0 | 38 | LEU |
| 10 | 0 | 41 | HIS |
| 10 | 0 | 45 | ASP |
| 10 | 0 | 51 | ARG |
| 10 | 0 | 53 | VAL |
| 10 | 0 | 56 | LYS |
| 11 | 4 | 3 | VAL |
| 11 | 4 | 9 | LYS |
| 11 | 4 | 12 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | 4 | 13 | ASN |
| 11 | 4 | 35 | GLN |
| 11 | 4 | 36 | ARG |
| 12 | 1 | 6 | GLU |
| 12 | 1 | 8 | ILE |
| 12 | 1 | 9 | LYS |
| 12 | 1 | 22 | THR |
| 12 | 1 | 34 | GLU |
| 12 | 1 | 35 | LEU |
| 12 | 1 | 43 | ARG |
| 12 | 1 | 44 | GLN |
| 13 | 3 | 7 | ARG |
| 13 | 3 | 14 | LYS |
| 13 | 3 | 18 | LYS |
| 13 | 3 | 27 | ASN |
| 13 | 3 | 42 | HIS |
| 14 | V | 18 | ARG |
| 14 | V | 40 | ILE |
| 14 | V | 42 | LEU |
| 14 | V | 46 | LYS |
| 14 | V | 51 | GLN |
| 14 | V | 53 | LYS |
| 14 | V | 55 | GLU |
| 14 | V | 66 | ASP |
| 14 | V | 70 | ILE |
| 14 | V | 75 | GLN |
| 14 | V | 79 | ARG |
| 14 | V | 86 | LEU |
| 14 | V | 89 | ILE |
| 14 | V | 90 | ASP |
| 14 | V | 93 | ARG |
| 15 | 2 | 10 | LEU |
| 15 | 2 | 19 | ARG |
| 15 | 2 | 21 | ARG |
| 15 | 2 | 24 | THR |
| 15 | 2 | 33 | ARG |
| 15 | 2 | 39 | ARG |
| 15 | 2 | 42 | LEU |
| 16 | L | 47 | ARG |
| 16 | L | 55 | MET |
| 16 | L | 69 | ARG |
| 16 | L | 77 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | L | 82 | LEU |
| 16 | L | 92 | LEU |
| 16 | L | 93 | ASN |
| 16 | L | 95 | LEU |
| 16 | L | 112 | LEU |
| 16 | L | 118 | THR |
| 16 | L | 123 | ARG |
| 17 | M | 10 | ARG |
| 17 | M | 30 | SER |
| 17 | M | 31 | PHE |
| 17 | M | 47 | GLU |
| 17 | M | 59 | ARG |
| 17 | M | 63 | ILE |
| 17 | M | 65 | ILE |
| 17 | M | 70 | ASP |
| 17 | M | 90 | GLU |
| 17 | M | 95 | LEU |
| 17 | M | 100 | LYS |
| 17 | M | 105 | MET |
| 17 | M | 108 | VAL |
| 17 | M | 110 | GLU |
| 17 | M | 115 | GLU |
| 17 | M | 127 | LYS |
| 18 | X | 18 | LEU |
| 18 | X | 28 | LEU |
| 18 | X | 29 | ARG |
| 18 | X | 48 | ARG |
| 18 | X | 49 | ASP |
| 18 | X | 59 | GLU |
| 19 | H | 1 | MET |
| 19 | H | 3 | VAL |
| 19 | H | 12 | LEU |
| 19 | H | 25 | TYR |
| 19 | H | 28 | ASN |
| 19 | H | 32 | PRO |
| 19 | H | 33 | GLN |
| 19 | H | 40 | THR |
| 19 | H | 45 | GLU |
| 19 | H | 70 | GLU |
| 19 | H | 75 | LEU |
| 19 | H | 83 | LYS |
| 19 | H | 89 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | H | 114 | GLU |
| 19 | H | 119 | ASN |
| 19 | H | 121 | VAL |
| 19 | H | 124 | THR |
| 19 | H | 125 | THR |
| 19 | H | 127 | GLU |
| 19 | H | 129 | GLU |
| 19 | H | 134 | VAL |
| 19 | H | 137 | GLU |
| 19 | H | 139 | PHE |
| 20 | J | 3 | THR |
| 20 | J | 5 | THR |
| 20 | J | 12 | LYS |
| 20 | J | 28 | LEU |
| 20 | J | 35 | ARG |
| 20 | J | 36 | LEU |
| 20 | J | 43 | GLU |
| 20 | J | 44 | TYR |
| 20 | J | 53 | TYR |
| 20 | J | 65 | THR |
| 20 | J | 69 | ARG |
| 20 | J | 73 | VAL |
| 20 | J | 76 | HIS |
| 20 | J | 95 | ARG |
| 20 | J | 111 | LYS |
| 20 | J | 122 | LEU |
| 20 | J | 124 | VAL |
| 20 | J | 129 | GLU |
| 21 | N | 1 | MET |
| 21 | N | 11 | ASN |
| 21 | N | 17 | ARG |
| 21 | N | 18 | GLN |
| 21 | N | 20 | MET |
| 21 | N | 35 | LYS |
| 21 | N | 48 | VAL |
| 21 | N | 69 | ARG |
| 21 | N | 71 | ARG |
| 21 | N | 82 | GLU |
| 21 | N | 98 | LEU |
| 21 | N | 112 | TYR |
| 21 | N | 114 | GLU |
| 21 | N | 118 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | O | 3 | LYS |
| 22 | O | 9 | ARG |
| 22 | O | 18 | LEU |
| 22 | O | 20 | GLU |
| 22 | O | 31 | THR |
| 22 | O | 36 | TYR |
| 22 | O | 58 | ILE |
| 22 | O | 62 | LEU |
| 22 | O | 67 | ASN |
| 22 | O | 74 | VAL |
| 22 | O | 78 | VAL |
| 22 | O | 91 | SER |
| 22 | O | 98 | GLN |
| 22 | O | 100 | HIS |
| 22 | O | 104 | GLN |
| 22 | O | 106 | LEU |
| 22 | O | 112 | GLU |
| 22 | O | 115 | LEU |
| 23 | Q | 5 | ARG |
| 23 | Q | 10 | ARG |
| 23 | Q | 13 | HIS |
| 23 | Q | 63 | ARG |
| 23 | Q | 79 | ILE |
| 23 | Q | 83 | LYS |
| 23 | Q | 90 | ASP |
| 23 | Q | 96 | ASP |
| 23 | Q | 105 | PHE |
| 24 | S | 6 | LYS |
| 24 | S | 7 | HIS |
| 24 | S | 15 | GLN |
| 24 | S | 18 | ARG |
| 24 | S | 22 | ASP |
| 24 | S | 31 | GLN |
| 24 | S | 33 | LEU |
| 24 | S | 45 | VAL |
| 24 | S | 62 | ASP |
| 24 | S | 66 | ILE |
| 24 | S | 73 | LYS |
| 24 | S | 84 | ARG |
| 24 | S | 86 | MET |
| 24 | S | 88 | ARG |
| 24 | S | 99 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | S | 101 | SER |
| 24 | S | 109 | ASP |
| 25 | U | 7 | ASP |
| 25 | U | 11 | ILE |
| 25 | U | 13 | LEU |
| 25 | U | 20 | LYS |
| 25 | U | 34 | ILE |
| 25 | U | 39 | ASN |
| 25 | U | 49 | PRO |
| 25 | U | 51 | LEU |
| 25 | U | 53 | GLN |
| 25 | U | 60 | LYS |
| 25 | U | 73 | ASN |
| 25 | U | 78 | LYS |
| 25 | U | 80 | ASP |
| 25 | U | 81 | ARG |
| 25 | U | 85 | ARG |
| 26 | F | 2 | LYS |
| 26 | F | 13 | LYS |
| 26 | F | 18 | GLU |
| 26 | F | 26 | GLN |
| 26 | F | 29 | ARG |
| 26 | F | 32 | LYS |
| 26 | F | 45 | ASP |
| 26 | F | 50 | ASP |
| 26 | F | 55 | ASP |
| 26 | F | 56 | LEU |
| 26 | F | 59 | ILE |
| 26 | F | 70 | ARG |
| 26 | F | 76 | PHE |
| 26 | F | 82 | TYR |
| 26 | F | 86 | CYS |
| 26 | F | 91 | ARG |
| 26 | F | 97 | GLU |
| 26 | F | 102 | LEU |
| 26 | F | 109 | ARG |
| 26 | F | 111 | ARG |
| 26 | F | 116 | LEU |
| 26 | F | 121 | PHE |
| 26 | F | 129 | MET |
| 26 | F | 133 | GLU |
| 26 | F | 134 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | F | 135 | ILE |
| 26 | F | 137 | PHE |
| 26 | F | 138 | PRO |
| 26 | F | 147 | ARG |
| 26 | F | 149 | ARG |
| 26 | F | 173 | ASP |
| 26 | F | 174 | PHE |
| 26 | F | 177 | ARG |
| 27 | G | 8 | VAL |
| 27 | G | 14 | VAL |
| 27 | G | 15 | ASP |
| 27 | G | 24 | THR |
| 27 | G | 31 | GLU |
| 27 | G | 34 | ARG |
| 27 | G | 54 | ARG |
| 27 | G | 61 | TRP |
| 27 | G | 68 | ARG |
| 27 | G | 70 | LEU |
| 27 | G | 71 | LEU |
| 27 | G | 74 | MET |
| 27 | G | 84 | LYS |
| 27 | G | 85 | LYS |
| 27 | G | 86 | LEU |
| 27 | G | 94 | ARG |
| 27 | G | 106 | LEU |
| 27 | G | 120 | ILE |
| 27 | G | 132 | LEU |
| 27 | G | 138 | GLN |
| 27 | G | 151 | ARG |
| 27 | G | 154 | GLU |
| 27 | G | 162 | ARG |
| 27 | G | 166 | GLU |
| 28 | R | 2 | TYR |
| 28 | R | 4 | VAL |
| 28 | R | 22 | LEU |
| 28 | R | 25 | LEU |
| 28 | R | 26 | ASP |
| 28 | R | 39 | LEU |
| 28 | R | 40 | MET |
| 28 | R | 45 | GLU |
| 28 | R | 48 | LYS |
| 28 | R | 70 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | R | 72 | VAL |
| 28 | R | 82 | HIS |
| 28 | R | 86 | GLN |
| 29 | T | 2 | ILE |
| 29 | T | 4 | GLU |
| 29 | T | 7 | LEU |
| 29 | T | 9 | LYS |
| 29 | T | 11 | LEU |
| 29 | T | 12 | ARG |
| 29 | T | 24 | MET |
| 29 | T | 32 | LEU |
| 29 | T | 64 | LYS |
| 29 | T | 68 | LYS |
| 29 | T | 73 | ARG |
| 29 | T | 87 | LEU |
| 30 | Z | 4 | VAL |
| 30 | Z | 14 | THR |
| 30 | Z | 18 | ARG |
| 30 | Z | 25 | THR |
| 30 | Z | 27 | ARG |
| 30 | Z | 32 | ASN |
| 30 | Z | 33 | LEU |
| 30 | Z | 37 | ARG |
| 30 | Z | 46 | PHE |
| 30 | Z | 49 | LEU |
| 30 | Z | 50 | ARG |
| 30 | Z | 66 | THR |
| 30 | Z | 78 | TYR |
| 31 | W | 10 | ARG |
| 31 | W | 14 | ASP |
| 31 | W | 18 | LYS |
| 31 | W | 19 | ARG |
| 31 | W | 23 | LYS |
| 31 | W | 24 | ARG |
| 31 | W | 25 | PHE |
| 31 | W | 38 | ARG |
| 31 | W | 39 | GLN |
| 31 | W | 40 | ARG |
| 31 | W | 44 | PHE |
| 31 | W | 49 | ASN |
| 31 | W | 50 | VAL |
| 31 | W | 74 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | W | 77 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 5 | GLN |
| 3 | I | 11 | GLN |
| 3 | I | 29 | GLN |
| 3 | I | 33 | ASN |
| 3 | I | 93 | ASN |
| 4 | C | 20 | ASN |
| 4 | C | 43 | ASN |
| 4 | C | 45 | ASN |
| 4 | C | 59 | GLN |
| 4 | C | 85 | ASN |
| 4 | C | 89 | ASN |
| 4 | C | 114 | GLN |
| 4 | C | 133 | ASN |
| 4 | C | 152 | GLN |
| 4 | C | 238 | ASN |
| 5 | D | 32 | ASN |
| 5 | D | 36 | GLN |
| 5 | D | 49 | GLN |
| 5 | D | 126 | ASN |
| 5 | D | 130 | GLN |
| 5 | D | 136 | ASN |
| 5 | D | 148 | GLN |
| 6 | K | 13 | ASN |
| 6 | K | 89 | ASN |
| 7 | P | 6 | GLN |
| 7 | P | 40 | GLN |
| 7 | P | 114 | ASN |
| 8 | E | 24 | ASN |
| 8 | E | 30 | GLN |
| 8 | E | 41 | GLN |
| 8 | E | 62 | GLN |
| 8 | E | 97 | ASN |
| 8 | E | 136 | GLN |
| 8 | E | 195 | GLN |
| 9 | Y | 33 | HIS |
| 9 | Y | 48 | ASN |
| 10 | 0 | 3 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | 4 | 13 | ASN |
| 11 | 4 | 35 | GLN |
| 12 | 1 | 25 | ASN |
| 13 | 3 | 42 | HIS |
| 14 | V | 44 | HIS |
| 14 | V | 49 | ASN |
| 14 | V | 51 | GLN |
| 14 | V | 80 | HIS |
| 15 | 2 | 16 | HIS |
| 16 | L | 4 | ASN |
| 16 | L | 54 | GLN |
| 16 | L | 93 | ASN |
| 16 | L | 104 | GLN |
| 17 | M | 3 | GLN |
| 17 | M | 13 | HIS |
| 17 | M | 17 | ASN |
| 18 | X | 15 | ASN |
| 18 | X | 20 | ASN |
| 18 | X | 25 | GLN |
| 18 | X | 31 | GLN |
| 18 | X | 41 | HIS |
| 19 | H | 18 | GLN |
| 19 | H | 28 | ASN |
| 19 | H | 66 | ASN |
| 19 | H | 145 | ASN |
| 20 | J | 40 | HIS |
| 20 | J | 138 | GLN |
| 21 | N | 11 | ASN |
| 21 | N | 107 | ASN |
| 22 | O | 19 | GLN |
| 22 | O | 38 | GLN |
| 22 | O | 61 | GLN |
| 22 | O | 67 | ASN |
| 23 | Q | 51 | GLN |
| 23 | Q | 70 | GLN |
| 23 | Q | 80 | ASN |
| 24 | S | 15 | GLN |
| 24 | S | 40 | ASN |
| 24 | S | 57 | ASN |
| 24 | S | 61 | ASN |
| 25 | U | 39 | ASN |
| 25 | U | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | U | 68 | ASN |
| 25 | U | 73 | ASN |
| 26 | F | 26 | GLN |
| 26 | F | 51 | ASN |
| 26 | F | 126 | ASN |
| 26 | F | 134 | GLN |
| 27 | G | 29 | ASN |
| 27 | G | 37 | ASN |
| 27 | G | 115 | GLN |
| 28 | R | 6 | GLN |
| 28 | R | 18 | GLN |
| 28 | R | 86 | GLN |
| 29 | T | 48 | GLN |
| 29 | T | 91 | GLN |
| 29 | T | 92 | ASN |
| 30 | Z | 23 | ASN |
| 30 | Z | 36 | HIS |
| 31 | W | 39 | GLN |
| 31 | W | 56 | HIS |
| 31 | W | 75 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 116/120 (96%) | 14 (12%) | 0 |
| 2 | B | 2837/2904 (97%) | 424 (14%) | 21 (0%) |
| All | All | 2953/3024 (97%) | 438 (14%) | 21 (0%) |

All (438) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | G |
| 1 | A | 15 | A |
| 1 | A | 16 | G |
| 1 | A | 26 | C |
| 1 | A | 29 | A |
| 1 | A | 30 | C |
| 1 | A | 35 | C |
| 1 | A | 42 | C |
| 1 | A | 43 | C |
| 1 | A | 67 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 88 | C |
| 1 | A | 90 | C |
| 1 | A | 99 | A |
| 1 | A | 109 | A |
| 2 | B | 11 | C |
| 2 | B | 33 | C |
| 2 | B | 34 | U |
| 2 | B | 46 | G |
| 2 | B | 51 | G |
| 2 | B | 63 | A |
| 2 | B | 64 | A |
| 2 | B | 71 | A |
| 2 | B | 74 | A |
| 2 | B | 75 | G |
| 2 | B | 84 | A |
| 2 | B | 99 | U |
| 2 | B | 100 | U |
| 2 | B | 101 | A |
| 2 | B | 102 | U |
| 2 | B | 103 | A |
| 2 | B | 119 | A |
| 2 | B | 120 | U |
| 2 | B | 125 | A |
| 2 | B | 126 | A |
| 2 | B | 139 | U |
| 2 | B | 140 | C |
| 2 | B | 141 | G |
| 2 | B | 142 | A |
| 2 | B | 143 | C |
| 2 | B | 160 | A |
| 2 | B | 162 | U |
| 2 | B | 163 | C |
| 2 | B | 174 | U |
| 2 | B | 181 | A |
| 2 | B | 196 | A |
| 2 | B | 199 | A |
| 2 | B | 215 | G |
| 2 | B | 216 | A |
| 2 | B | 221 | A |
| 2 | B | 222 | A |
| 2 | B | 233 | A |
| 2 | B | 248 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 252 | G |
| 2 | B | 255 | A |
| 2 | B | 265 | A |
| 2 | B | 266 | G |
| 2 | B | 267 | C |
| 2 | B | 271 | G |
| 2 | B | 277 | G |
| 2 | B | 278 | A |
| 2 | B | 280 | U |
| 2 | B | 281 | C |
| 2 | B | 282 | A |
| 2 | B | 284 | U |
| 2 | B | 287 | G |
| 2 | B | 288 | U |
| 2 | B | 289 | G |
| 2 | B | 295 | G |
| 2 | B | 311 | A |
| 2 | B | 323 | C |
| 2 | B | 329 | G |
| 2 | B | 330 | A |
| 2 | B | 347 | A |
| 2 | B | 349 | U |
| 2 | B | 350 | G |
| 2 | B | 352 | A |
| 2 | B | 354 | A |
| 2 | B | 356 | G |
| 2 | B | 357 | C |
| 2 | B | 358 | U |
| 2 | B | 363 | G |
| 2 | B | 371 | A |
| 2 | B | 372 | G |
| 2 | B | 383 | C |
| 2 | B | 386 | G |
| 2 | B | 387 | U |
| 2 | B | 396 | G |
| 2 | B | 411 | G |
| 2 | B | 423 | A |
| 2 | B | 424 | G |
| 2 | B | 444 | C |
| 2 | B | 451 | U |
| 2 | B | 455 | C |
| 2 | B | 456 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 457 | A |
| 2 | B | 473 | G |
| 2 | B | 479 | A |
| 2 | B | 480 | A |
| 2 | B | 481 | G |
| 2 | B | 491 | G |
| 2 | B | 504 | A |
| 2 | B | 505 | A |
| 2 | B | 508 | A |
| 2 | B | 509 | C |
| 2 | B | 510 | C |
| 2 | B | 512 | G |
| 2 | B | 527 | C |
| 2 | B | 531 | C |
| 2 | B | 532 | A |
| 2 | B | 533 | G |
| 2 | B | 542 | C |
| 2 | B | 544 | C |
| 2 | B | 545 | U |
| 2 | B | 546 | U |
| 2 | B | 547 | A |
| 2 | B | 548 | G |
| 2 | B | 549 | G |
| 2 | B | 550 | C |
| 2 | B | 563 | A |
| 2 | B | 573 | U |
| 2 | B | 575 | A |
| 2 | B | 603 | A |
| 2 | B | 613 | A |
| 2 | B | 614 | A |
| 2 | B | 615 | U |
| 2 | B | 616 | A |
| 2 | B | 627 | A |
| 2 | B | 632 | A |
| 2 | B | 637 | A |
| 2 | B | 645 | C |
| 2 | B | 646 | U |
| 2 | B | 653 | U |
| 2 | B | 654 | A |
| 2 | B | 655 | A |
| 2 | B | 671 | C |
| 2 | B | 686 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 699 | A |
| 2 | B | 717 | C |
| 2 | B | 718 | A |
| 2 | B | 719 | C |
| 2 | B | 722 | A |
| 2 | B | 730 | A |
| 2 | B | 747 | U |
| 2 | B | 765 | C |
| 2 | B | 775 | G |
| 2 | B | 782 | A |
| 2 | B | 784 | G |
| 2 | B | 785 | G |
| 2 | B | 805 | G |
| 2 | B | 811 | U |
| 2 | B | 812 | C |
| 2 | B | 819 | A |
| 2 | B | 827 | U |
| 2 | B | 828 | U |
| 2 | B | 846 | U |
| 2 | B | 847 | U |
| 2 | B | 859 | G |
| 2 | B | 869 | G |
| 2 | B | 876 | C |
| 2 | B | 899 | A |
| 2 | B | 903 | C |
| 2 | B | 910 | A |
| 2 | B | 912 | C |
| 2 | B | 931 | U |
| 2 | B | 932 | U |
| 2 | B | 933 | A |
| 2 | B | 941 | A |
| 2 | B | 946 | C |
| 2 | B | 953 | G |
| 2 | B | 955 | U |
| 2 | B | 961 | C |
| 2 | B | 973 | A |
| 2 | B | 974 | G |
| 2 | B | 983 | A |
| 2 | B | 991 | C |
| 2 | B | 995 | C |
| 2 | B | 996 | A |
| 2 | B | 1012 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1013 | C |
| 2 | B | 1022 | G |
| 2 | B | 1025 | G |
| 2 | B | 1033 | U |
| 2 | B | 1042 | G |
| 2 | B | 1046 | A |
| 2 | B | 1047 | G |
| 2 | B | 1070 | A |
| 2 | B | 1088 | A |
| 2 | B | 1090 | A |
| 2 | B | 1098 | A |
| 2 | B | 1111 | A |
| 2 | B | 1112 | G |
| 2 | B | 1116 | G |
| 2 | B | 1126 | A |
| 2 | B | 1127 | A |
| 2 | B | 1132 | U |
| 2 | B | 1133 | A |
| 2 | B | 1134 | A |
| 2 | B | 1135 | C |
| 2 | B | 1136 | G |
| 2 | B | 1142 | A |
| 2 | B | 1143 | A |
| 2 | B | 1176 | U |
| 2 | B | 1195 | G |
| 2 | B | 1204 | A |
| 2 | B | 1205 | A |
| 2 | B | 1206 | G |
| 2 | B | 1211 | C |
| 2 | B | 1212 | G |
| 2 | B | 1237 | A |
| 2 | B | 1241 | A |
| 2 | B | 1242 | U |
| 2 | B | 1247 | A |
| 2 | B | 1248 | G |
| 2 | B | 1253 | A |
| 2 | B | 1256 | G |
| 2 | B | 1266 | G |
| 2 | B | 1271 | G |
| 2 | B | 1272 | A |
| 2 | B | 1273 | U |
| 2 | B | 1275 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1276 | A |
| 2 | B | 1301 | A |
| 2 | B | 1302 | A |
| 2 | B | 1325 | U |
| 2 | B | 1337 | G |
| 2 | B | 1341 | G |
| 2 | B | 1365 | A |
| 2 | B | 1368 | G |
| 2 | B | 1379 | U |
| 2 | B | 1383 | A |
| 2 | B | 1384 | A |
| 2 | B | 1396 | U |
| 2 | B | 1397 | U |
| 2 | B | 1416 | G |
| 2 | B | 1419 | A |
| 2 | B | 1420 | A |
| 2 | B | 1427 | A |
| 2 | B | 1428 | C |
| 2 | B | 1434 | A |
| 2 | B | 1451 | C |
| 2 | B | 1453 | A |
| 2 | B | 1454 | C |
| 2 | B | 1459 | G |
| 2 | B | 1460 | U |
| 2 | B | 1461 | C |
| 2 | B | 1470 | A |
| 2 | B | 1476 | U |
| 2 | B | 1477 | A |
| 2 | B | 1482 | G |
| 2 | B | 1493 | C |
| 2 | B | 1504 | A |
| 2 | B | 1507 | C |
| 2 | B | 1508 | A |
| 2 | B | 1509 | A |
| 2 | B | 1510 | G |
| 2 | B | 1512 | C |
| 2 | B | 1524 | G |
| 2 | B | 1531 | C |
| 2 | B | 1536 | C |
| 2 | B | 1540 | G |
| 2 | B | 1552 | A |
| 2 | B | 1558 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1559 | U |
| 2 | B | 1567 | G |
| 2 | B | 1569 | A |
| 2 | B | 1578 | U |
| 2 | B | 1583 | A |
| 2 | B | 1584 | U |
| 2 | B | 1585 | C |
| 2 | B | 1600 | C |
| 2 | B | 1603 | A |
| 2 | B | 1608 | A |
| 2 | B | 1610 | A |
| 2 | B | 1634 | A |
| 2 | B | 1635 | A |
| 2 | B | 1640 | A |
| 2 | B | 1647 | U |
| 2 | B | 1648 | U |
| 2 | B | 1674 | G |
| 2 | B | 1700 | A |
| 2 | B | 1703 | G |
| 2 | B | 1713 | A |
| 2 | B | 1715 | G |
| 2 | B | 1716 | U |
| 2 | B | 1730 | C |
| 2 | B | 1731 | G |
| 2 | B | 1733 | G |
| 2 | B | 1738 | G |
| 2 | B | 1756 | G |
| 2 | B | 1764 | C |
| 2 | B | 1772 | A |
| 2 | B | 1773 | A |
| 2 | B | 1800 | C |
| 2 | B | 1816 | C |
| 2 | B | 1829 | A |
| 2 | B | 1870 | C |
| 2 | B | 1872 | A |
| 2 | B | 1884 | G |
| 2 | B | 1906 | G |
| 2 | B | 1912 | A |
| 2 | B | 1913 | A |
| 2 | B | 1914 | C |
| 2 | B | 1927 | A |
| 2 | B | 1929 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1930 | G |
| 2 | B | 1938 | A |
| 2 | B | 1939 | U |
| 2 | B | 1940 | U |
| 2 | B | 1955 | U |
| 2 | B | 1967 | C |
| 2 | B | 1970 | A |
| 2 | B | 1971 | U |
| 2 | B | 1972 | G |
| 2 | B | 1991 | U |
| 2 | B | 1993 | U |
| 2 | B | 1997 | C |
| 2 | B | 2020 | A |
| 2 | B | 2022 | U |
| 2 | B | 2023 | C |
| 2 | B | 2031 | A |
| 2 | B | 2033 | A |
| 2 | B | 2043 | C |
| 2 | B | 2055 | C |
| 2 | B | 2056 | G |
| 2 | B | 2060 | A |
| 2 | B | 2061 | G |
| 2 | B | 2062 | A |
| 2 | B | 2069 | G |
| 2 | B | 2076 | U |
| 2 | B | 2093 | G |
| 2 | B | 2096 | C |
| 2 | B | 2099 | U |
| 2 | B | 2107 | G |
| 2 | B | 2108 | A |
| 2 | B | 2109 | U |
| 2 | B | 2110 | G |
| 2 | B | 2135 | A |
| 2 | B | 2138 | G |
| 2 | B | 2145 | C |
| 2 | B | 2147 | A |
| 2 | B | 2148 | G |
| 2 | B | 2156 | G |
| 2 | B | 2157 | G |
| 2 | B | 2180 | U |
| 2 | B | 2188 | U |
| 2 | B | 2190 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 2193 | G |
| 2 | B | 2198 | A |
| 2 | B | 2203 | U |
| 2 | B | 2204 | G |
| 2 | B | 2211 | A |
| 2 | B | 2212 | A |
| 2 | B | 2225 | A |
| 2 | B | 2238 | G |
| 2 | B | 2239 | G |
| 2 | B | 2268 | A |
| 2 | B | 2283 | C |
| 2 | B | 2287 | A |
| 2 | B | 2288 | A |
| 2 | B | 2297 | A |
| 2 | B | 2305 | U |
| 2 | B | 2307 | G |
| 2 | B | 2308 | G |
| 2 | B | 2311 | A |
| 2 | B | 2320 | U |
| 2 | B | 2321 | U |
| 2 | B | 2322 | A |
| 2 | B | 2325 | G |
| 2 | B | 2333 | A |
| 2 | B | 2335 | A |
| 2 | B | 2336 | A |
| 2 | B | 2337 | G |
| 2 | B | 2345 | G |
| 2 | B | 2347 | C |
| 2 | B | 2361 | G |
| 2 | B | 2379 | G |
| 2 | B | 2383 | G |
| 2 | B | 2385 | C |
| 2 | B | 2388 | A |
| 2 | B | 2396 | G |
| 2 | B | 2402 | U |
| 2 | B | 2406 | A |
| 2 | B | 2423 | U |
| 2 | B | 2424 | C |
| 2 | B | 2426 | A |
| 2 | B | 2429 | G |
| 2 | B | 2430 | A |
| 2 | B | 2434 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 2441 | U |
| 2 | B | 2448 | A |
| 2 | B | 2472 | G |
| 2 | B | 2476 | A |
| 2 | B | 2491 | U |
| 2 | B | 2502 | G |
| 2 | B | 2505 | G |
| 2 | B | 2506 | U |
| 2 | B | 2518 | A |
| 2 | B | 2535 | G |
| 2 | B | 2554 | U |
| 2 | B | 2566 | A |
| 2 | B | 2567 | G |
| 2 | B | 2573 | C |
| 2 | B | 2586 | U |
| 2 | B | 2602 | A |
| 2 | B | 2609 | U |
| 2 | B | 2613 | U |
| 2 | B | 2629 | U |
| 2 | B | 2634 | A |
| 2 | B | 2654 | A |
| 2 | B | 2682 | A |
| 2 | B | 2689 | U |
| 2 | B | 2690 | U |
| 2 | B | 2714 | G |
| 2 | B | 2726 | A |
| 2 | B | 2744 | G |
| 2 | B | 2748 | A |
| 2 | B | 2757 | A |
| 2 | B | 2760 | C |
| 2 | B | 2778 | A |
| 2 | B | 2791 | G |
| 2 | B | 2796 | U |
| 2 | B | 2797 | U |
| 2 | B | 2799 | A |
| 2 | B | 2800 | A |
| 2 | B | 2801 | G |
| 2 | B | 2802 | G |
| 2 | B | 2808 | G |
| 2 | B | 2820 | A |
| 2 | B | 2821 | A |
| 2 | B | 2836 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 2850 | A |
| 2 | B | 2866 | U |
| 2 | B | 2867 | G |
| 2 | B | 2872 | A |
| 2 | B | 2873 | A |
| 2 | B | 2883 | A |
| 2 | B | 2894 | G |
| 2 | B | 2903 | U |

All (21) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 63 | A |
| 2 | B | 125 | A |
| 2 | B | 162 | U |
| 2 | B | 508 | A |
| 2 | B | 544 | C |
| 2 | B | 670 | A |
| 2 | B | 1126 | A |
| 2 | B | 1205 | A |
| 2 | B | 1210 | G |
| 2 | B | 1301 | A |
| 2 | B | 1419 | A |
| 2 | B | 1911 | U |
| 2 | B | 2282 | G |
| 2 | B | 2324 | U |
| 2 | B | 2336 | A |
| 2 | B | 2425 | A |
| 2 | B | 2434 | A |
| 2 | B | 2756 | U |
| 2 | B | 2798 | U |
| 2 | B | 2873 | A |
| 2 | B | 2894 | G |

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 113 ligands modelled in this entry, 112 are monoatomic - leaving 1 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 | $\# Z > 2$ |
| 34 | LLL | B | 3619 | - | 33,33,33 | 3.19 | 14 (42%) | 49,49,49 | 1.48 | 6 (12%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 34 | LLL | B | 3619 | - | - | 0/12/65/65 | 0/3/3/3 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 34 | B | 3619 | LLL | C22-C32 | 8.92 | 1.59 | 1.52 |
| 34 | B | 3619 | LLL | C22-C12 | 7.45 | 1.58 | 1.52 |
| 34 | B | 3619 | LLL | O53-C53 | 6.07 | 1.52 | 1.43 |
| 34 | B | 3619 | LLL | C43-C33 | 4.96 | 1.63 | 1.54 |
| 34 | B | 3619 | LLL | C42-C32 | 4.78 | 1.59 | 1.52 |
| 34 | B | 3619 | LLL | O53-C13 | 4.48 | 1.51 | 1.41 |
| 34 | B | 3619 | LLL | C53-C43 | 3.79 | 1.56 | 1.52 |
| 34 | B | 3619 | LLL | O51-C11 | 3.70 | 1.51 | 1.41 |
| 34 | B | 3619 | LLL | C41-C51 | 3.46 | 1.60 | 1.51 |
| 34 | B | 3619 | LLL | C23-C33 | 2.81 | 1.60 | 1.52 |
| 34 | B | 3619 | LLL | C52-C42 | 2.67 | 1.60 | 1.52 |
| 34 | B | 3619 | LLL | C31-C21 | 2.41 | 1.59 | 1.52 |
| 34 | B | 3619 | LLL | C52-C62 | 2.18 | 1.58 | 1.52 |
| 34 | B | 3619 | LLL | C62-C12 | 2.06 | 1.55 | 1.52 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34 | B | 3619 | LLL | C93-N33-C33 | 5.90 | 117.21 | 113.85 |
| 34 | B | 3619 | LLL | C53-O53-C13 | 4.50 | 117.63 | 111.22 |
| 34 | B | 3619 | LLL | C83-C43-C33 | 2.73 | 116.68 | 112.15 |
| 34 | B | 3619 | LLL | O43-C43-C83 | -2.52 | 102.51 | 108.08 |
| 34 | B | 3619 | LLL | C11-O51-C51 | 2.02 | 115.23 | 113.19 |
| 34 | B | 3619 | LLL | C13-O62-C62 | 2.00 | 123.10 | 117.99 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 117/120 (97%) | 0.13 | 9 (7%) 13 7 | 30, 80, 115, 155 | 0 |
| 2 | B | 2841/2904 (97%) | 0.17 | 213 (7%) 14 7 | 5, 45, 124, 163 | 0 |
| 3 | I | 141/141 (100%) | -0.50 | 0 100 100 | 70, 117, 148, 160 | 0 |
| 4 | C | 271/272 (99%) | 0.16 | 19 (7%) 16 8 | 5, 32, 80, 112 | 0 |
| 5 | D | 209/209 (100%) | 0.14 | 8 (3%) 38 18 | 5, 49, 98, 135 | 0 |
| 6 | K | 121/123 (98%) | 1.55 | 42 (34%) 1 1 | 5, 37, 90, 130 | 0 |
| 7 | P | 114/114 (100%) | 0.45 | 14 (12%) 5 4 | 7, 49, 94, 112 | 0 |
| 8 | E | 201/201 (100%) | -0.18 | 5 (2%) 54 26 | 5, 62, 107, 138 | 0 |
| 9 | Y | 58/58 (100%) | 0.52 | 9 (15%) 3 3 | 6, 64, 110, 117 | 0 |
| 10 | 0 | 56/56 (100%) | 0.07 | 3 (5%) 25 11 | 10, 43, 99, 104 | 0 |
| 11 | 4 | 38/38 (100%) | 0.18 | 1 (2%) 53 25 | 15, 65, 94, 105 | 0 |
| 12 | 1 | 50/54 (92%) | -0.19 | 0 100 100 | 27, 74, 105, 118 | 0 |
| 13 | 3 | 64/64 (100%) | 1.09 | 14 (21%) 1 2 | 5, 39, 84, 101 | 0 |
| 14 | V | 94/94 (100%) | -0.06 | 4 (4%) 34 15 | 8, 79, 108, 125 | 0 |
| 15 | 2 | 46/46 (100%) | 1.32 | 14 (30%) 1 1 | 5, 28, 69, 113 | 0 |
| 16 | L | 143/144 (99%) | 0.44 | 18 (12%) 4 3 | 5, 55, 95, 123 | 0 |
| 17 | M | 136/136 (100%) | 0.22 | 9 (6%) 18 9 | 5, 55, 94, 134 | 0 |
| 18 | X | 63/63 (100%) | -0.36 | 0 100 100 | 36, 82, 107, 142 | 0 |
| 19 | H | 149/149 (100%) | -0.47 | 0 100 100 | 18, 88, 112, 141 | 0 |
| 20 | J | 142/142 (100%) | 0.17 | 9 (6%) 19 9 | 5, 60, 101, 131 | 0 |
| 21 | N | 120/127 (94%) | -0.05 | 5 (4%) 35 15 | 5, 42, 75, 118 | 0 |
| 22 | O | 116/117 (99%) | 0.59 | 20 (17%) 2 2 | 5, 73, 106, 157 | 0 |
| 23 | Q | 117/117 (100%) | 0.42 | 13 (11%) 6 4 | 5, 50, 92, 120 | 0 |
| 24 | S | 110/110 (100%) | 0.22 | 5 (4%) 32 14 | 5, 48, 95, 128 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 25 | U | 102/103 (99%) | -0.04 | 5 (4%) 28 13 | 34, 80, 112, 130 | 0 |
| 26 | F | 178/178 (100%) | 0.06 | 9 (5%) 27 12 | 38, 85, 125, 138 | 0 |
| 27 | G | 176/176 (100%) | 0.02 | 9 (5%) 27 12 | 17, 82, 110, 133 | 0 |
| 28 | R | 103/103 (100%) | -0.21 | 0 100 100 | 15, 72, 111, 128 | 0 |
| 29 | T | 93/100 (93%) | 0.33 | 5 (5%) 25 11 | 8, 66, 108, 120 | 0 |
| 30 | Z | 77/78 (98%) | 0.03 | 3 (3%) 37 17 | 5, 43, 87, 114 | 0 |
| 31 | W | 79/84 (94%) | 0.59 | 8 (10%) 7 5 | 12, 65, 103, 122 | 0 |
| All | All | 6325/6421 (98%) | 0.17 | 473 (7%) 14 7 | 5, 55, 118, 163 | 0 |

All (473) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 645 | C | 12.3 |
| 1 | A | 88 | C | 10.6 |
| 6 | K | 110 | GLU | 8.3 |
| 22 | O | 3 | LYS | 8.0 |
| 2 | B | 350 | G | 7.7 |
| 2 | B | 504 | A | 7.6 |
| 6 | K | 111 | LYS | 7.1 |
| 2 | B | 1459 | G | 7.0 |
| 9 | Y | 1 | ALA | 6.9 |
| 2 | B | 284 | U | 6.7 |
| 2 | B | 952 | G | 6.7 |
| 2 | B | 2547 | A | 6.7 |
| 2 | B | 2213 | U | 6.6 |
| 2 | B | 2272 | U | 6.6 |
| 7 | P | 36 | LYS | 6.5 |
| 2 | B | 351 | C | 6.5 |
| 1 | A | 118 | C | 6.4 |
| 2 | B | 349 | U | 6.3 |
| 9 | Y | 2 | LYS | 6.1 |
| 2 | B | 436 | C | 6.1 |
| 2 | B | 953 | G | 6.1 |
| 2 | B | 54 | G | 6.0 |
| 2 | B | 31 | C | 5.9 |
| 24 | S | 110 | ARG | 5.9 |
| 23 | Q | 84 | LYS | 5.9 |
| 1 | A | 89 | U | 5.8 |
| 26 | F | 177 | ARG | 5.8 |
| 2 | B | 43 | G | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 508 | A | 5.7 |
| 2 | B | 1148 | U | 5.6 |
| 2 | B | 2357 | G | 5.6 |
| 2 | B | 2273 | A | 5.6 |
| 2 | B | 30 | G | 5.6 |
| 7 | P | 33 | GLU | 5.5 |
| 2 | B | 2764 | A | 5.5 |
| 6 | K | 108 | ARG | 5.4 |
| 20 | J | 44 | TYR | 5.3 |
| 27 | G | 57 | TYR | 5.3 |
| 2 | B | 2524 | G | 5.3 |
| 17 | M | 59 | ARG | 5.3 |
| 2 | B | 2566 | A | 5.2 |
| 23 | Q | 4 | LYS | 5.2 |
| 2 | B | 282 | A | 5.2 |
| 2 | B | 1490 | A | 5.1 |
| 2 | B | 1241 | A | 4.9 |
| 2 | B | 283 | G | 4.9 |
| 29 | T | 56 | GLU | 4.8 |
| 2 | B | 2356 | U | 4.7 |
| 26 | F | 178 | LYS | 4.7 |
| 2 | B | 331 | C | 4.7 |
| 2 | B | 285 | G | 4.7 |
| 2 | B | 472 | A | 4.7 |
| 2 | B | 244 | A | 4.6 |
| 2 | B | 2423 | U | 4.6 |
| 2 | B | 968 | C | 4.5 |
| 2 | B | 1847 | A | 4.5 |
| 2 | B | 1045 | C | 4.5 |
| 20 | J | 10 | THR | 4.5 |
| 2 | B | 2191 | A | 4.5 |
| 2 | B | 2523 | G | 4.4 |
| 2 | B | 1535 | A | 4.4 |
| 23 | Q | 5 | ARG | 4.4 |
| 21 | N | 120 | GLU | 4.4 |
| 2 | B | 456 | C | 4.4 |
| 26 | F | 124 | ARG | 4.4 |
| 31 | W | 16 | GLU | 4.3 |
| 2 | B | 1460 | U | 4.3 |
| 2 | B | 2190 | G | 4.3 |
| 22 | O | 2 | ASP | 4.3 |
| 23 | Q | 117 | ALA | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 582 | A | 4.3 |
| 2 | B | 28 | A | 4.3 |
| 2 | B | 2189 | U | 4.3 |
| 2 | B | 53 | A | 4.3 |
| 2 | B | 513 | A | 4.2 |
| 17 | M | 38 | ARG | 4.2 |
| 4 | C | 34 | GLU | 4.2 |
| 1 | A | 85 | G | 4.2 |
| 2 | B | 2424 | C | 4.2 |
| 6 | K | 18 | ARG | 4.2 |
| 2 | B | 56 | A | 4.1 |
| 2 | B | 437 | U | 4.1 |
| 2 | B | 1530 | G | 4.1 |
| 26 | F | 93 | GLU | 4.1 |
| 2 | B | 2227 | A | 4.1 |
| 22 | O | 60 | GLU | 4.1 |
| 4 | C | 268 | ARG | 4.1 |
| 5 | D | 120 | GLY | 4.1 |
| 2 | B | 44 | A | 4.0 |
| 26 | F | 115 | GLY | 4.0 |
| 2 | B | 52 | A | 4.0 |
| 2 | B | 965 | C | 4.0 |
| 2 | B | 967 | U | 3.9 |
| 23 | Q | 55 | GLN | 3.9 |
| 27 | G | 110 | HIS | 3.9 |
| 2 | B | 2463 | C | 3.9 |
| 9 | Y | 58 | GLU | 3.9 |
| 6 | K | 112 | PHE | 3.9 |
| 2 | B | 101 | A | 3.8 |
| 2 | B | 1046 | A | 3.8 |
| 22 | O | 57 | ALA | 3.8 |
| 2 | B | 455 | C | 3.8 |
| 2 | B | 2422 | C | 3.8 |
| 14 | V | 82 | TYR | 3.8 |
| 2 | B | 2799 | A | 3.8 |
| 2 | B | 2271 | G | 3.8 |
| 2 | B | 29 | U | 3.8 |
| 2 | B | 2734 | A | 3.8 |
| 4 | C | 1 | ALA | 3.7 |
| 26 | F | 2 | LYS | 3.7 |
| 16 | L | 51 | GLU | 3.7 |
| 2 | B | 1260 | A | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 2797 | U | 3.7 |
| 23 | Q | 115 | ALA | 3.7 |
| 8 | E | 56 | GLY | 3.7 |
| 2 | B | 245 | G | 3.7 |
| 2 | B | 1859 | U | 3.6 |
| 2 | B | 438 | G | 3.6 |
| 2 | B | 2790 | U | 3.6 |
| 2 | B | 2358 | A | 3.6 |
| 10 | 0 | 55 | ALA | 3.6 |
| 15 | 2 | 40 | ALA | 3.6 |
| 2 | B | 458 | G | 3.6 |
| 2 | B | 1283 | G | 3.6 |
| 2 | B | 1666 | G | 3.5 |
| 31 | W | 14 | ASP | 3.5 |
| 4 | C | 260 | LYS | 3.5 |
| 2 | B | 46 | G | 3.5 |
| 2 | B | 471 | A | 3.5 |
| 2 | B | 1147 | A | 3.5 |
| 31 | W | 42 | THR | 3.5 |
| 6 | K | 38 | ILE | 3.5 |
| 2 | B | 100 | U | 3.5 |
| 2 | B | 1458 | U | 3.5 |
| 2 | B | 1870 | C | 3.5 |
| 7 | P | 35 | SER | 3.5 |
| 2 | B | 32 | C | 3.5 |
| 2 | B | 42 | A | 3.5 |
| 22 | O | 21 | LEU | 3.5 |
| 17 | M | 16 | ARG | 3.5 |
| 2 | B | 102 | U | 3.5 |
| 2 | B | 794 | A | 3.4 |
| 6 | K | 8 | LEU | 3.4 |
| 2 | B | 948 | C | 3.4 |
| 15 | 2 | 1 | MET | 3.4 |
| 2 | B | 1026 | G | 3.4 |
| 6 | K | 27 | GLY | 3.4 |
| 17 | M | 1 | MET | 3.4 |
| 6 | K | 25 | LEU | 3.4 |
| 2 | B | 435 | C | 3.4 |
| 5 | D | 104 | VAL | 3.4 |
| 2 | B | 2672 | U | 3.4 |
| 2 | B | 180 | G | 3.4 |
| 31 | W | 13 | ARG | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 23 | Q | 21 | LYS | 3.4 |
| 23 | Q | 10 | ARG | 3.3 |
| 2 | B | 949 | G | 3.3 |
| 2 | B | 2395 | C | 3.3 |
| 1 | A | 86 | G | 3.3 |
| 5 | D | 103 | ASP | 3.3 |
| 2 | B | 2757 | A | 3.3 |
| 2 | B | 405 | U | 3.3 |
| 2 | B | 2265 | U | 3.3 |
| 2 | B | 1253 | A | 3.3 |
| 6 | K | 3 | GLN | 3.2 |
| 31 | W | 17 | ALA | 3.2 |
| 2 | B | 1216 | G | 3.2 |
| 6 | K | 107 | LEU | 3.2 |
| 22 | O | 116 | GLN | 3.2 |
| 2 | B | 947 | A | 3.2 |
| 13 | 3 | 16 | THR | 3.2 |
| 6 | K | 113 | MET | 3.2 |
| 13 | 3 | 15 | LYS | 3.2 |
| 13 | 3 | 19 | GLY | 3.2 |
| 2 | B | 959 | A | 3.2 |
| 7 | P | 87 | ARG | 3.2 |
| 6 | K | 105 | ARG | 3.2 |
| 22 | O | 61 | GLN | 3.2 |
| 2 | B | 2275 | C | 3.2 |
| 7 | P | 105 | LYS | 3.2 |
| 24 | S | 27 | LYS | 3.2 |
| 7 | P | 102 | ARG | 3.1 |
| 22 | O | 20 | GLU | 3.1 |
| 22 | O | 63 | LYS | 3.1 |
| 2 | B | 1254 | A | 3.1 |
| 2 | B | 359 | G | 3.1 |
| 17 | M | 37 | GLY | 3.1 |
| 16 | L | 69 | ARG | 3.1 |
| 6 | K | 22 | ILE | 3.1 |
| 15 | 2 | 39 | ARG | 3.1 |
| 2 | B | 489 | G | 3.1 |
| 16 | L | 47 | ARG | 3.1 |
| 2 | B | 809 | G | 3.1 |
| 6 | K | 7 | MET | 3.1 |
| 6 | K | 33 | ALA | 3.1 |
| 7 | P | 34 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | K | 20 | MET | 3.1 |
| 4 | C | 263 | ASP | 3.1 |
| 20 | J | 43 | GLU | 3.0 |
| 21 | N | 118 | ARG | 3.0 |
| 4 | C | 53 | ILE | 3.0 |
| 2 | B | 34 | U | 3.0 |
| 6 | K | 39 | ILE | 3.0 |
| 24 | S | 26 | GLY | 3.0 |
| 2 | B | 583 | G | 3.0 |
| 2 | B | 2188 | U | 3.0 |
| 22 | O | 89 | ASP | 3.0 |
| 10 | 0 | 54 | ILE | 3.0 |
| 2 | B | 179 | C | 3.0 |
| 2 | B | 55 | G | 3.0 |
| 6 | K | 21 | CYS | 3.0 |
| 16 | L | 60 | ARG | 3.0 |
| 2 | B | 1532 | A | 3.0 |
| 2 | B | 512 | G | 2.9 |
| 2 | B | 566 | U | 2.9 |
| 31 | W | 43 | LYS | 2.9 |
| 6 | K | 4 | GLU | 2.9 |
| 14 | V | 83 | LYS | 2.9 |
| 2 | B | 473 | G | 2.9 |
| 2 | B | 795 | C | 2.9 |
| 2 | B | 2255 | G | 2.9 |
| 2 | B | 1451 | C | 2.9 |
| 2 | B | 2568 | U | 2.9 |
| 6 | K | 30 | ARG | 2.9 |
| 13 | 3 | 18 | LYS | 2.9 |
| 2 | B | 1027 | A | 2.9 |
| 2 | B | 2194 | U | 2.9 |
| 7 | P | 101 | GLU | 2.9 |
| 2 | B | 41 | C | 2.9 |
| 2 | B | 1219 | U | 2.9 |
| 9 | Y | 3 | THR | 2.9 |
| 7 | P | 38 | ARG | 2.9 |
| 13 | 3 | 14 | LYS | 2.9 |
| 31 | W | 40 | ARG | 2.9 |
| 2 | B | 474 | G | 2.9 |
| 9 | Y | 57 | GLU | 2.9 |
| 2 | B | 1044 | C | 2.8 |
| 15 | 2 | 31 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 1281 | G | 2.8 |
| 2 | B | 1542 | U | 2.8 |
| 25 | U | 87 | GLU | 2.8 |
| 13 | 3 | 51 | LYS | 2.8 |
| 5 | D | 85 | ALA | 2.8 |
| 22 | O | 24 | THR | 2.8 |
| 16 | L | 65 | GLY | 2.8 |
| 2 | B | 196 | A | 2.8 |
| 2 | B | 969 | G | 2.8 |
| 2 | B | 1345 | C | 2.8 |
| 15 | 2 | 33 | ARG | 2.8 |
| 2 | B | 1540 | G | 2.8 |
| 16 | L | 67 | THR | 2.8 |
| 2 | B | 47 | C | 2.8 |
| 2 | B | 946 | C | 2.8 |
| 2 | B | 1808 | A | 2.8 |
| 2 | B | 1858 | A | 2.8 |
| 4 | C | 2 | VAL | 2.8 |
| 7 | P | 40 | GLN | 2.8 |
| 6 | K | 44 | LYS | 2.8 |
| 20 | J | 11 | VAL | 2.8 |
| 6 | K | 29 | HIS | 2.8 |
| 2 | B | 139 | U | 2.7 |
| 2 | B | 2192 | U | 2.7 |
| 15 | 2 | 46 | LYS | 2.7 |
| 27 | G | 171 | LYS | 2.7 |
| 2 | B | 1382 | G | 2.7 |
| 29 | T | 71 | GLY | 2.7 |
| 29 | T | 72 | GLN | 2.7 |
| 13 | 3 | 63 | TYR | 2.7 |
| 2 | B | 2147 | A | 2.7 |
| 1 | A | 90 | C | 2.7 |
| 2 | B | 1531 | C | 2.7 |
| 5 | D | 1 | MET | 2.7 |
| 27 | G | 172 | GLU | 2.7 |
| 2 | B | 509 | C | 2.7 |
| 8 | E | 55 | SER | 2.7 |
| 23 | Q | 8 | ILE | 2.7 |
| 2 | B | 2193 | G | 2.7 |
| 2 | B | 565 | C | 2.7 |
| 6 | K | 92 | GLU | 2.7 |
| 16 | L | 50 | PHE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | G | 173 | ALA | 2.7 |
| 22 | O | 88 | LYS | 2.7 |
| 2 | B | 1217 | U | 2.7 |
| 16 | L | 63 | LYS | 2.7 |
| 29 | T | 42 | GLU | 2.7 |
| 2 | B | 2266 | A | 2.7 |
| 2 | B | 546 | U | 2.7 |
| 2 | B | 577 | G | 2.7 |
| 2 | B | 1210 | G | 2.7 |
| 1 | A | 87 | U | 2.6 |
| 2 | B | 251 | A | 2.6 |
| 16 | L | 92 | LEU | 2.6 |
| 2 | B | 453 | A | 2.6 |
| 16 | L | 49 | GLY | 2.6 |
| 2 | B | 1449 | G | 2.6 |
| 6 | K | 35 | VAL | 2.6 |
| 9 | Y | 56 | VAL | 2.6 |
| 2 | B | 2732 | G | 2.6 |
| 15 | 2 | 37 | LYS | 2.6 |
| 22 | O | 56 | LYS | 2.6 |
| 2 | B | 543 | G | 2.6 |
| 2 | B | 2602 | A | 2.6 |
| 26 | F | 173 | ASP | 2.6 |
| 2 | B | 2394 | C | 2.6 |
| 2 | B | 348 | A | 2.6 |
| 5 | D | 74 | GLU | 2.6 |
| 6 | K | 37 | ASP | 2.6 |
| 2 | B | 145 | C | 2.6 |
| 2 | B | 2794 | C | 2.6 |
| 25 | U | 36 | GLU | 2.6 |
| 2 | B | 57 | C | 2.6 |
| 6 | K | 24 | VAL | 2.6 |
| 20 | J | 12 | LYS | 2.5 |
| 5 | D | 166 | GLY | 2.5 |
| 2 | B | 1215 | G | 2.5 |
| 2 | B | 2359 | C | 2.5 |
| 2 | B | 1259 | G | 2.5 |
| 2 | B | 1617 | C | 2.5 |
| 2 | B | 1242 | U | 2.5 |
| 6 | K | 93 | GLN | 2.5 |
| 15 | 2 | 42 | LEU | 2.5 |
| 2 | B | 1381 | G | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | B | 2567 | G | 2.5 |
| 9 | Y | 38 | GLU | 2.5 |
| 2 | B | 2462 | C | 2.5 |
| 27 | G | 56 | GLY | 2.5 |
| 6 | K | 109 | SER | 2.5 |
| 4 | C | 3 | VAL | 2.5 |
| 2 | B | 1149 | G | 2.5 |
| 16 | L | 10 | GLU | 2.5 |
| 22 | O | 62 | LEU | 2.5 |
| 2 | B | 1280 | G | 2.4 |
| 7 | P | 61 | ARG | 2.4 |
| 31 | W | 41 | GLY | 2.4 |
| 15 | 2 | 35 | ARG | 2.4 |
| 16 | L | 58 | TYR | 2.4 |
| 13 | 3 | 49 | VAL | 2.4 |
| 6 | K | 34 | GLY | 2.4 |
| 2 | B | 578 | G | 2.4 |
| 2 | B | 2667 | C | 2.4 |
| 14 | V | 55 | GLU | 2.4 |
| 4 | C | 169 | ALA | 2.4 |
| 22 | O | 58 | ILE | 2.4 |
| 9 | Y | 10 | ARG | 2.4 |
| 13 | 3 | 13 | PHE | 2.4 |
| 2 | B | 252 | G | 2.4 |
| 2 | B | 2260 | C | 2.4 |
| 25 | U | 90 | LYS | 2.4 |
| 23 | Q | 19 | GLN | 2.4 |
| 30 | Z | 28 | ARG | 2.4 |
| 2 | B | 514 | A | 2.4 |
| 23 | Q | 6 | GLY | 2.4 |
| 29 | T | 70 | HIS | 2.4 |
| 7 | P | 88 | ARG | 2.4 |
| 13 | 3 | 7 | ARG | 2.4 |
| 2 | B | 1284 | A | 2.4 |
| 23 | Q | 85 | ALA | 2.4 |
| 4 | C | 213 | ARG | 2.4 |
| 13 | 3 | 22 | LYS | 2.4 |
| 26 | F | 94 | ARG | 2.4 |
| 2 | B | 1869 | G | 2.4 |
| 2 | B | 2733 | A | 2.4 |
| 22 | O | 84 | GLU | 2.3 |
| 6 | K | 45 | GLU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | K | 84 | CYS | 2.3 |
| 7 | P | 37 | LYS | 2.3 |
| 4 | C | 22 | GLU | 2.3 |
| 2 | B | 1731 | G | 2.3 |
| 2 | B | 2609 | U | 2.3 |
| 2 | B | 1450 | G | 2.3 |
| 2 | B | 1702 | G | 2.3 |
| 4 | C | 229 | HIS | 2.3 |
| 2 | B | 26 | G | 2.3 |
| 25 | U | 86 | PHE | 2.3 |
| 30 | Z | 77 | LYS | 2.3 |
| 2 | B | 1537 | G | 2.3 |
| 2 | B | 2256 | G | 2.3 |
| 2 | B | 961 | C | 2.3 |
| 2 | B | 205 | G | 2.3 |
| 16 | L | 52 | GLY | 2.3 |
| 2 | B | 1030 | C | 2.3 |
| 6 | K | 26 | GLY | 2.3 |
| 6 | K | 71 | ARG | 2.3 |
| 6 | K | 9 | ASN | 2.3 |
| 2 | B | 567 | U | 2.3 |
| 13 | 3 | 64 | ALA | 2.3 |
| 23 | Q | 20 | ALA | 2.3 |
| 17 | M | 18 | ARG | 2.3 |
| 21 | N | 32 | GLU | 2.3 |
| 15 | 2 | 6 | GLN | 2.3 |
| 16 | L | 54 | GLN | 2.3 |
| 2 | B | 1533 | C | 2.3 |
| 16 | L | 57 | LEU | 2.3 |
| 2 | B | 352 | A | 2.2 |
| 22 | O | 112 | GLU | 2.2 |
| 16 | L | 117 | THR | 2.2 |
| 15 | 2 | 38 | GLY | 2.2 |
| 2 | B | 1463 | C | 2.2 |
| 6 | K | 104 | THR | 2.2 |
| 20 | J | 45 | THR | 2.2 |
| 17 | M | 15 | GLY | 2.2 |
| 2 | B | 515 | A | 2.2 |
| 2 | B | 1134 | A | 2.2 |
| 2 | B | 1175 | A | 2.2 |
| 17 | M | 19 | GLY | 2.2 |
| 4 | C | 209 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | K | 40 | LYS | 2.2 |
| 14 | V | 10 | LYS | 2.2 |
| 2 | B | 511 | U | 2.2 |
| 8 | E | 54 | GLY | 2.2 |
| 2 | B | 291 | G | 2.2 |
| 4 | C | 21 | PRO | 2.2 |
| 4 | C | 5 | CYS | 2.2 |
| 24 | S | 28 | LYS | 2.2 |
| 20 | J | 4 | PHE | 2.2 |
| 22 | O | 22 | GLY | 2.2 |
| 2 | B | 1240 | U | 2.2 |
| 4 | C | 204 | LEU | 2.2 |
| 16 | L | 48 | ARG | 2.2 |
| 20 | J | 51 | GLY | 2.2 |
| 6 | K | 5 | GLN | 2.2 |
| 1 | A | 99 | A | 2.2 |
| 6 | K | 83 | ALA | 2.2 |
| 15 | 2 | 36 | ALA | 2.2 |
| 15 | 2 | 32 | ALA | 2.1 |
| 13 | 3 | 60 | CYS | 2.1 |
| 2 | B | 749 | A | 2.1 |
| 9 | Y | 55 | LYS | 2.1 |
| 5 | D | 128 | ARG | 2.1 |
| 2 | B | 631 | A | 2.1 |
| 2 | B | 1465 | G | 2.1 |
| 11 | 4 | 20 | ASP | 2.1 |
| 2 | B | 960 | A | 2.1 |
| 25 | U | 25 | LYS | 2.1 |
| 26 | F | 105 | ILE | 2.1 |
| 22 | O | 114 | GLY | 2.1 |
| 2 | B | 457 | A | 2.1 |
| 2 | B | 1464 | G | 2.1 |
| 30 | Z | 29 | PHE | 2.1 |
| 2 | B | 644 | A | 2.1 |
| 24 | S | 82 | MET | 2.1 |
| 16 | L | 59 | ARG | 2.1 |
| 2 | B | 358 | U | 2.1 |
| 2 | B | 2082 | A | 2.1 |
| 10 | 0 | 56 | LYS | 2.1 |
| 15 | 2 | 41 | ARG | 2.1 |
| 2 | B | 1995 | U | 2.1 |
| 4 | C | 15 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 98 | G | 2.1 |
| 2 | B | 1119 | U | 2.1 |
| 7 | P | 107 | ALA | 2.1 |
| 2 | B | 353 | C | 2.1 |
| 2 | B | 490 | C | 2.1 |
| 2 | B | 2771 | C | 2.1 |
| 6 | K | 23 | LYS | 2.1 |
| 22 | O | 115 | LEU | 2.1 |
| 4 | C | 17 | LYS | 2.0 |
| 8 | E | 53 | THR | 2.0 |
| 27 | G | 168 | VAL | 2.0 |
| 21 | N | 110 | MET | 2.0 |
| 6 | K | 28 | SER | 2.0 |
| 21 | N | 119 | SER | 2.0 |
| 2 | B | 12 | U | 2.0 |
| 4 | C | 40 | GLY | 2.0 |
| 6 | K | 66 | LYS | 2.0 |
| 27 | G | 58 | ALA | 2.0 |
| 8 | E | 51 | GLU | 2.0 |
| 27 | G | 9 | VAL | 2.0 |
| 13 | 3 | 20 | GLY | 2.0 |
| 20 | J | 37 | ARG | 2.0 |
| 2 | B | 1252 | G | 2.0 |
| 2 | B | 1541 | C | 2.0 |
| 17 | M | 60 | GLN | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 32 | MG | B | 3452 | 1/1 | 0.33 | 14.67 | 50,50,50,50 | 0 |
| 32 | MG | B | 3337 | 1/1 | 0.37 | 13.41 | 96,96,96,96 | 0 |
| 32 | MG | B | 3279 | 1/1 | 0.63 | 10.55 | 36,36,36,36 | 0 |
| 34 | LLL | B | 3619 | 31/31 | 0.25 | 9.38 | 54,54,54,54 | 0 |
| 32 | MG | B | 3165 | 1/1 | 1.10 | 5.74 | 37,37,37,37 | 0 |
| 32 | MG | B | 3515 | 1/1 | 1.45 | 5.47 | 57,57,57,57 | 0 |
| 32 | MG | B | 3262 | 1/1 | 0.25 | 5.17 | 66,66,66,66 | 0 |
| 32 | MG | B | 3207 | 1/1 | 0.98 | 3.34 | 54,54,54,54 | 0 |
| 32 | MG | B | 3201 | 1/1 | 0.41 | 2.61 | 74,74,74,74 | 0 |
| 32 | MG | B | 3351 | 1/1 | 0.23 | 1.53 | 79,79,79,79 | 0 |
| 32 | MG | B | 3274 | 1/1 | 0.30 | 1.43 | 5,5,5,5 | 0 |
| 32 | MG | B | 3570 | 1/1 | 0.23 | 1.23 | 26,26,26,26 | 0 |
| 32 | MG | B | 3184 | 1/1 | 0.24 | 0.86 | 8,8,8,8 | 0 |
| 32 | MG | B | 3087 | 1/1 | 0.15 | 0.79 | 50,50,50,50 | 0 |
| 32 | MG | B | 3409 | 1/1 | 0.28 | 0.74 | 21,21,21,21 | 0 |
| 32 | MG | B | 3457 | 1/1 | 0.28 | 0.51 | 48,48,48,48 | 0 |
| 32 | MG | B | 3618 | 1/1 | 0.31 | 0.51 | 43,43,43,43 | 0 |
| 32 | MG | B | 3592 | 1/1 | 0.17 | 0.51 | 37,37,37,37 | 0 |
| 32 | MG | B | 3419 | 1/1 | 0.28 | 0.17 | 34,34,34,34 | 0 |
| 32 | MG | B | 3239 | 1/1 | 0.30 | 0.03 | 41,41,41,41 | 0 |
| 32 | MG | B | 3021 | 1/1 | 0.24 | -0.27 | 21,21,21,21 | 0 |
| 32 | MG | B | 3301 | 1/1 | 0.48 | -0.32 | 62,62,62,62 | 0 |
| 32 | MG | B | 3257 | 1/1 | 0.37 | -0.35 | 18,18,18,18 | 0 |
| 32 | MG | B | 3598 | 1/1 | 0.36 | -0.47 | 15,15,15,15 | 0 |
| 32 | MG | B | 3220 | 1/1 | 0.17 | -0.48 | 5,5,5,5 | 0 |
| 32 | MG | B | 3033 | 1/1 | 0.15 | -0.52 | 5,5,5,5 | 0 |
| 32 | MG | B | 3127 | 1/1 | 0.15 | -0.58 | 23,23,23,23 | 0 |
| 32 | MG | B | 3001 | 1/1 | 0.14 | -0.73 | 5,5,5,5 | 0 |
| 32 | MG | B | 3069 | 1/1 | 0.19 | -0.74 | 14,14,14,14 | 0 |
| 32 | MG | B | 3320 | 1/1 | 0.27 | -0.83 | 11,11,11,11 | 0 |
| 32 | MG | B | 3357 | 1/1 | 0.15 | -0.84 | 58,58,58,58 | 0 |
| 32 | MG | B | 3525 | 1/1 | 0.11 | -0.86 | 76,76,76,76 | 0 |
| 32 | MG | B | 3104 | 1/1 | 0.16 | -0.89 | 48,48,48,48 | 0 |
| 32 | MG | B | 3172 | 1/1 | 0.15 | -0.91 | 66,66,66,66 | 0 |
| 32 | MG | B | 3547 | 1/1 | 0.17 | -0.95 | 42,42,42,42 | 0 |
| 32 | MG | B | 3544 | 1/1 | 0.12 | -0.97 | 5,5,5,5 | 0 |
| 32 | MG | B | 3485 | 1/1 | 0.17 | -0.98 | 56,56,56,56 | 0 |
| 32 | MG | B | 3537 | 1/1 | 0.13 | -0.99 | 96,96,96,96 | 0 |
| 32 | MG | B | 3308 | 1/1 | 0.18 | -1.04 | 66,66,66,66 | 0 |
| 32 | MG | B | 3492 | 1/1 | 0.16 | -1.05 | 25,25,25,25 | 0 |
| 32 | MG | B | 3564 | 1/1 | 0.11 | -1.06 | 5,5,5,5 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 32 | MG | B | 3026 | 1/1 | 0.13 | -1.17 | 6,6,6,6 | 0 |
| 32 | MG | B | 3140 | 1/1 | 0.14 | -1.21 | 53,53,53,53 | 0 |
| 32 | MG | B | 3081 | 1/1 | 0.10 | -1.21 | 13,13,13,13 | 0 |
| 32 | MG | B | 3189 | 1/1 | 0.16 | -1.23 | 45,45,45,45 | 0 |
| 32 | MG | B | 3327 | 1/1 | 0.16 | -1.26 | 5,5,5,5 | 0 |
| 33 | ZN | 4 | 624 | 1/1 | 0.06 | -1.30 | 45,45,45,45 | 0 |
| 32 | MG | B | 3008 | 1/1 | 0.13 | -1.32 | 12,12,12,12 | 0 |
| 32 | MG | B | 3225 | 1/1 | 0.16 | -1.39 | 17,17,17,17 | 0 |
| 32 | MG | B | 3614 | 1/1 | 0.08 | -1.39 | 29,29,29,29 | 0 |
| 32 | MG | B | 3052 | 1/1 | 0.11 | -1.43 | 5,5,5,5 | 0 |
| 32 | MG | B | 3474 | 1/1 | 0.23 | -1.45 | 5,5,5,5 | 0 |
| 32 | MG | B | 3040 | 1/1 | 0.09 | -1.49 | 18,18,18,18 | 0 |
| 32 | MG | B | 3196 | 1/1 | 0.08 | -1.51 | 18,18,18,18 | 0 |
| 32 | MG | B | 3064 | 1/1 | 0.09 | -1.63 | 35,35,35,35 | 0 |
| 32 | MG | B | 3584 | 1/1 | 0.10 | -1.74 | 55,55,55,55 | 0 |
| 32 | MG | B | 3152 | 1/1 | 0.13 | -1.76 | 33,33,33,33 | 0 |
| 32 | MG | B | 3332 | 1/1 | 0.07 | -1.79 | 53,53,53,53 | 0 |
| 32 | MG | B | 3292 | 1/1 | 0.03 | -1.80 | 73,73,73,73 | 0 |
| 32 | MG | B | 3446 | 1/1 | 0.11 | -1.81 | 43,43,43,43 | 0 |
| 32 | MG | B | 3440 | 1/1 | 0.08 | -1.82 | 41,41,41,41 | 0 |
| 32 | MG | B | 3370 | 1/1 | 0.09 | -1.84 | 21,21,21,21 | 0 |
| 32 | MG | B | 3074 | 1/1 | 0.14 | -1.89 | 37,37,37,37 | 0 |
| 32 | MG | B | 3214 | 1/1 | 0.09 | -1.89 | 26,26,26,26 | 0 |
| 32 | MG | B | 3413 | 1/1 | 0.14 | -1.94 | 43,43,43,43 | 0 |
| 32 | MG | B | 3298 | 1/1 | 0.07 | -1.96 | 57,57,57,57 | 0 |
| 32 | MG | B | 3268 | 1/1 | 0.10 | -2.04 | 5,5,5,5 | 0 |
| 32 | MG | B | 3463 | 1/1 | 0.09 | -2.05 | 43,43,43,43 | 0 |
| 32 | MG | B | 3559 | 1/1 | 0.07 | -2.07 | 5,5,5,5 | 0 |
| 32 | MG | B | 3058 | 1/1 | 0.29 | -2.09 | 14,14,14,14 | 0 |
| 32 | MG | B | 3480 | 1/1 | 0.09 | -2.10 | 42,42,42,42 | 0 |
| 32 | MG | B | 3382 | 1/1 | 0.07 | -2.15 | 16,16,16,16 | 0 |
| 32 | MG | B | 3512 | 1/1 | 0.07 | -2.19 | 52,52,52,52 | 0 |
| 32 | MG | B | 3014 | 1/1 | 0.12 | -2.22 | 17,17,17,17 | 0 |
| 32 | MG | B | 3425 | 1/1 | 0.15 | -2.24 | 25,25,25,25 | 0 |
| 32 | MG | B | 3532 | 1/1 | 0.12 | -2.24 | 14,14,14,14 | 0 |
| 32 | MG | B | 3528 | 1/1 | 0.10 | -2.26 | 7,7,7,7 | 0 |
| 32 | MG | B | 3179 | 1/1 | 0.11 | -2.45 | 26,26,26,26 | 0 |
| 32 | MG | B | 3504 | 1/1 | 0.08 | -2.52 | 63,63,63,63 | 0 |
| 32 | MG | B | 3496 | 1/1 | 0.09 | -2.54 | 5,5,5,5 | 0 |
| 32 | MG | B | 3235 | 1/1 | 0.05 | -2.63 | 5,5,5,5 | 0 |
| 32 | MG | B | 3117 | 1/1 | 0.09 | -2.64 | 5,5,5,5 | 0 |
| 32 | MG | B | 3245 | 1/1 | 0.08 | -2.65 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|-----------------------------|-------|
| 32 | MG | B | 3375 | 1/1 | 0.07 | -2.82 | 11,11,11,11 | 0 |
| 32 | MG | B | 3468 | 1/1 | 0.10 | -2.86 | 5,5,5,5 | 0 |
| 32 | MG | B | 3575 | 1/1 | 0.05 | -3.08 | 16,16,16,16 | 0 |
| 32 | MG | B | 3092 | 1/1 | 0.13 | -3.16 | 17,17,17,17 | 0 |
| 32 | MG | B | 3099 | 1/1 | 0.08 | -3.23 | 5,5,5,5 | 0 |
| 32 | MG | B | 3344 | 1/1 | 0.10 | -3.29 | 100,100,100,100 | 0 |
| 32 | MG | B | 3315 | 1/1 | 0.06 | -3.32 | 13,13,13,13 | 0 |
| 32 | MG | B | 3553 | 1/1 | 0.07 | -3.34 | 23,23,23,23 | 0 |
| 32 | MG | B | 3436 | 1/1 | 0.07 | -3.34 | 5,5,5,5 | 0 |
| 32 | MG | B | 3251 | 1/1 | 0.08 | -3.43 | 5,5,5,5 | 0 |
| 32 | MG | B | 3521 | 1/1 | 0.07 | -3.51 | 45,45,45,45 | 0 |
| 32 | MG | B | 3579 | 1/1 | 0.09 | -3.54 | 7,7,7,7 | 0 |
| 32 | MG | B | 3396 | 1/1 | 0.12 | -3.57 | 5,5,5,5 | 0 |
| 32 | MG | B | 3403 | 1/1 | 0.09 | -3.73 | 5,5,5,5 | 0 |
| 32 | MG | B | 3431 | 1/1 | 0.09 | -3.74 | 33,33,33,33 | 0 |
| 32 | MG | B | 3286 | 1/1 | 0.06 | -3.79 | 5,5,5,5 | 0 |
| 32 | MG | B | 3133 | 1/1 | 0.15 | -3.83 | 13,13,13,13 | 0 |
| 32 | MG | B | 3602 | 1/1 | 0.06 | -3.84 | 5,5,5,5 | 0 |
| 32 | MG | B | 3146 | 1/1 | 0.07 | -4.16 | 5,5,5,5 | 0 |
| 32 | MG | B | 3500 | 1/1 | 0.07 | -4.17 | 24,24,24,24 | 0 |
| 32 | MG | B | 3229 | 1/1 | 0.05 | -4.24 | 36,36,36,36 | 0 |
| 32 | MG | B | 3110 | 1/1 | 0.08 | -4.40 | 6,6,6,6 | 0 |
| 32 | MG | B | 3364 | 1/1 | 0.04 | -4.64 | 43,43,43,43 | 0 |
| 32 | MG | B | 3609 | 1/1 | 0.15 | -4.68 | 28,28,28,28 | 0 |
| 32 | MG | B | 3508 | 1/1 | 0.06 | -5.69 | 18,18,18,18 | 0 |
| 32 | MG | B | 3122 | 1/1 | 0.07 | -5.78 | 5,5,5,5 | 0 |
| 32 | MG | B | 3159 | 1/1 | 0.06 | -6.15 | 12,12,12,12 | 0 |
| 32 | MG | B | 3588 | 1/1 | 0.11 | -7.38 | 30,30,30,30 | 0 |
| 32 | MG | B | 3046 | 1/1 | 0.09 | -10.43 | 8,8,8,8 | 0 |
| 32 | MG | B | 3389 | 1/1 | 0.42 | - | 100,100,100,100 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.