



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:11 PM BST

PDB ID : 3JAH  
EMDB ID: : EMD-3039  
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAG stop codon  
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.  
Deposited on : 2015-06-10  
Resolution : 3.45 Å(reported)  
Based on PDB ID : 1DT9, 4V51, 3J7P, 3J92, 3BK7

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

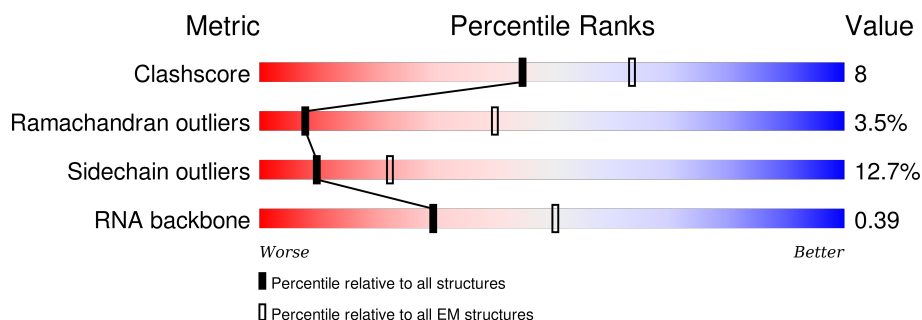
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.45 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.






















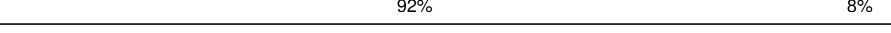





| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |
| RNA backbone          | 3027                        | 244                         |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 244    | 76% 18% 5%       |
| 2   | B     | 394    | 76% 21% .        |
| 3   | C     | 362    | 71% 26% .        |
| 4   | D     | 292    | 79% 18% .        |
| 5   | E     | 248    | 65% 25% 5% 5%    |
| 6   | F     | 225    | 76% 20% . .      |
| 7   | G     | 241    | 78% 22% .        |
| 8   | H     | 190    | 81% 17% .        |














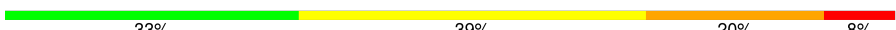


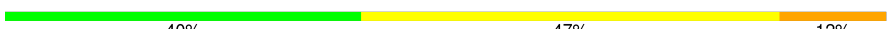
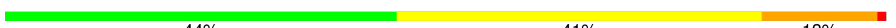







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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | I     | 213    |    |
| 10  | J     | 169    |    |
| 11  | L     | 210    |    |
| 12  | M     | 138    |    |
| 13  | N     | 203    |    |
| 14  | O     | 199    |    |
| 15  | P     | 153    |    |
| 16  | Q     | 187    |    |
| 17  | R     | 180    |    |
| 18  | S     | 175    |    |
| 19  | T     | 159    |    |
| 20  | U     | 99     |   |
| 21  | V     | 131    |  |
| 22  | W     | 63     |  |
| 23  | X     | 119    |  |
| 24  | Y     | 134    |  |
| 25  | Z     | 135    |  |
| 26  | a     | 147    |  |
| 27  | b     | 75     |  |
| 28  | c     | 94     |  |
| 29  | d     | 107    |  |
| 30  | e     | 128    |  |
| 31  | f     | 109    |  |
| 32  | g     | 114    |  |
| 33  | h     | 122    |  |


























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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 34  | i     | 102    |  91% 9%           |
| 35  | j     | 86     |  83% 15%          |
| 36  | k     | 69     |  84% 14%          |
| 37  | l     | 50     |  84% 16%          |
| 38  | m     | 52     |  83% 17%          |
| 39  | n     | 23     |  83% 17%          |
| 40  | o     | 104    |  86% 13%          |
| 41  | p     | 91     |  92% 8%           |
| 42  | r     | 125    |  78% 18%          |
| 43  | s     | 198    |  90% 10%          |
| 44  | t     | 163    |  80% 20%          |
| 45  | 1     | 15     |  73% 20% 7%      |
| 46  | 2     | 76     |  59% 32% 8%     |
| 47  | 3     | 75     |  33% 39% 20% 8% |
| 48  | 5     | 3662   |  46% 40% 13%    |
| 49  | 7     | 120    |  63% 32% 5%     |
| 50  | 8     | 156    |  40% 47% 12%    |
| 51  | 9     | 1719   |  44% 41% 13%    |
| 52  | AA    | 208    |  70% 28%        |
| 53  | BB    | 213    |  73% 23%        |
| 54  | CC    | 218    |  74% 23%        |
| 55  | DD    | 227    |  81% 18%        |
| 56  | EE    | 262    |  65% 27% 7%     |
| 57  | FF    | 191    |  68% 28%        |
| 58  | GG    | 237    |  75% 21% 5%     |





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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 59  | HH    | 189    |  71% 24% 5%     |
| 60  | II    | 206    |  69% 30% .      |
| 61  | JJ    | 185    |  75% 18% 6% .   |
| 62  | KK    | 98     |  71% 27% .      |
| 63  | LL    | 152    |  70% 24% . .    |
| 64  | MM    | 124    |  75% 24% .      |
| 65  | NN    | 150    |  76% 22% .      |
| 66  | OO    | 136    |  67% 23% 7% .   |
| 67  | PP    | 127    |  75% 21% .      |
| 68  | QQ    | 141    |  77% 20% .      |
| 69  | RR    | 129    |  78% 19% .      |
| 70  | SS    | 137    |  74% 20% . .   |
| 71  | TT    | 141    |  79% 16% 5% . |
| 72  | UU    | 104    |  75% 22% . .  |
| 73  | VV    | 83     |  73% 24% .    |
| 74  | WW    | 129    |  65% 29% 5% . |
| 75  | XX    | 141    |  72% 23% 5%   |
| 76  | YY    | 126    |  73% 22% 5%   |
| 77  | ZZ    | 75     |  77% 23%      |
| 78  | aa    | 98     |  81% 19%      |
| 79  | bb    | 83     |  80% 20%      |
| 80  | cc    | 61     |  80% 20%      |
| 81  | dd    | 53     |  81% 19%      |
| 82  | ee    | 57     |  82% 16% .    |
| 83  | ff    | 68     |  87% . 9%     |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 84  | gg    | 313    | <br>90% 9%   |
| 85  | hh    | 12     | <br>42% 58%  |
| 86  | ii    | 416    | <br>89% 10%  |
| 87  | jj    | 594    | <br>91% 5% • |

## 2 Entry composition [i](#)

There are 91 unique types of molecules in this entry. The entry contains 226454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1868  | 1171 | 382 | 309 | 6 |         |       |

- Molecule 2 is a protein called uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3148  | 2007 | 591 | 537 | 13 |         |       |

- Molecule 3 is a protein called uL4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2884  | 1814 | 578 | 478 | 14 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 361     | LYS      | -      | EXPRESSION TAG | UNP G1SVW5 |
| C     | 362     | LYS      | -      | EXPRESSION TAG | UNP G1SVW5 |
| C     | 363     | SER      | -      | EXPRESSION TAG | UNP G1SVW5 |

- Molecule 4 is a protein called uL18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 292      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2386  | 1509 | 437 | 426 | 14 |         |       |

- Molecule 5 is a protein called eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1215 | 362 | 318 | 3 |         |       |

- Molecule 6 is a protein called uL30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | F     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 7 is a protein called eL8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | G     | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1934  | 1233 | 371 | 326 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| G     | 191     | GLY      | CYS    | CONFLICT | UNP G1STW0 |

- Molecule 8 is a protein called uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 954 | 284 | 272 | 6 |         |       |

- Molecule 9 is a protein called uL16.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | I     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1655  | 1051 | 319 | 272 | 13 |         |       |

- Molecule 10 is a protein called uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1353  | 855 | 252 | 240 | 6 |         |       |

- Molecule 11 is a protein called eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | L     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1703  | 1065 | 354 | 280 | 4 |         |       |

- Molecule 12 is a protein called eL14.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | M     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1137  | 727 | 221 | 182 | 7 |         |       |

- Molecule 13 is a protein called eL15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | N     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 14 is a protein called uL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | O     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1638  | 1056 | 321 | 256 | 5 |         |       |

- Molecule 15 is a protein called uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | P     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 16 is a protein called uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Q     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 941 | 311 | 249 | 5 |         |       |

- Molecule 17 is a protein called eL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | R     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 933 | 328 | 238 | 9 |         |       |

- Molecule 18 is a protein called eL20.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18  | S     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1454  | 925 | 284 | 235 | 10 |         |       |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | T     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 20 is a protein called eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | U     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 518 | 141 | 147 | 2 |         |       |

- Molecule 21 is a protein called uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | V     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 22 is a protein called eL24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 22  | W     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 528   | 337 | 103 | 85 | 3 |         |       |

- Molecule 23 is a protein called uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | X     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 976   | 624 | 183 | 168 | 1 |         |       |

- Molecule 24 is a protein called uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Y     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 25 is a protein called eL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Z     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 26 is a protein called uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | a     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 734 | 239 | 185 | 4 |         |       |

- Molecule 27 is a protein called eL29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | b     | 75       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 609   | 378 | 130 | 98 | 3 |         |       |

- Molecule 28 is a protein called eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 732   | 465 | 130 | 131 | 6 |         |       |

- Molecule 29 is a protein called eL31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 30 is a protein called eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 31 is a protein called eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 143 | 4 |         |       |

- Molecule 32 is a protein called eL34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 33 is a protein called uL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 640 | 204 | 168 | 1 |         |       |

- Molecule 34 is a protein called eL36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 520 | 176 | 129 | 5 |         |       |

- Molecule 35 is a protein called eL37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | j     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 36 is a protein called eL38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | k     | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37  | l     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 38 is a protein called eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | m     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 39 is a protein called eL41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | n     | 23       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 222   | 134 | 61 | 25 | 2 |         |       |

- Molecule 40 is a protein called eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 851   | 533 | 174 | 138 | 6 |         |       |

- Molecule 41 is a protein called eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | p     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 42 is a protein called eL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | r     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1001  | 621 | 206 | 168 | 6 |         |       |

- Molecule 43 is a protein called uL10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | s     | 198      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1523  | 969 | 265 | 280 | 9 |         |       |

- Molecule 44 is a protein called uL11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | t     | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1238  | 773 | 230 | 230 | 5 |         |       |

- Molecule 45 is a protein called peptide.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 45  | 1     | 15       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 125   | 82 | 20 | 22 | 1 |         |       |

- Molecule 46 is a RNA chain called tRNA(Val).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 46  | 2     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1616  | 723 | 291 | 527 | 75 |         |       |

- Molecule 47 is a RNA chain called tRNA(Lys).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 47  | 3     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1593  | 712 | 281 | 526 | 74 |         |       |

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 48  | 5     | 3662     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 78486 | 34947 | 14363 | 25515 | 3661 |         |       |

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 49  | 7     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 50  | 8     | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3314  | 1480 | 585 | 1094 | 155 |         |       |

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 51  | 9     | 1719     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36680 | 16371 | 6586 | 12005 | 1718 |         |       |

- Molecule 52 is a protein called uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | AA    | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1045 | 289 | 300 | 8 |         |       |

- Molecule 53 is a protein called eS1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | BB    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1729  | 1098 | 309 | 308 | 14 |         |       |

- Molecule 54 is a protein called uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | CC    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1692  | 1102 | 287 | 296 | 7 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| CC    | 194     | ARG      | HIS    | CONFLICT | UNP G1TUT9 |
| CC    | 228     | GLY      | SER    | CONFLICT | UNP G1TUT9 |

- Molecule 55 is a protein called uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | DD    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1124 | 317 | 315 | 8 |         |       |

- Molecule 56 is a protein called eS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | EE    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2073  | 1323 | 384 | 357 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| EE    | 25      | GLY      | SER    | CONFLICT | UNP G1TK17 |

- Molecule 57 is a protein called uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | FF    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1509  | 943 | 286 | 273 | 7 |         |       |

- Molecule 58 is a protein called eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 58  | GG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 59 is a protein called eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | HH    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1521  | 969 | 280 | 271 | 1 |         |       |

- Molecule 60 is a protein called eS8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | II    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| II    | 47      | ARG      | GLY    | CONFLICT | UNP G1TJW1 |

- Molecule 61 is a protein called uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | JJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 62 is a protein called eS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | KK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |

- Molecule 63 is a protein called uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | LL    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1238  | 788 | 232 | 212 | 6 |         |       |

- Molecule 64 is a protein called eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | MM    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 600 | 170 | 179 | 9 |         |       |

- Molecule 65 is a protein called uS15.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | NN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 66 is a protein called uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | OO    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 621 | 199 | 190 | 6 |         |       |

- Molecule 67 is a protein called uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | PP    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1060  | 673 | 201 | 179 | 7 |         |       |

- Molecule 68 is a protein called uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | QQ    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 715 | 212 | 194 | 3 |         |       |

- Molecule 69 is a protein called eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | RR    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 658 | 193 | 191 | 5 |         |       |

- Molecule 70 is a protein called uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SS    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1139  | 714 | 231 | 193 | 1 |         |       |

- Molecule 71 is a protein called eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | TT    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 692 | 212 | 195 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| TT    | 119     | GLY      | TRP    | CONFLICT | UNP G1TN62 |

- Molecule 72 is a protein called uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | UU    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |

- Molecule 73 is a protein called eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | VV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 394 | 118 | 119 | 5 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| VV    | 3       | ASN      | SER    | CONFLICT | UNP G1TM82 |
| VV    | 4       | ASP      | ASN    | CONFLICT | UNP G1TM82 |
| VV    | 50      | PHE      | SER    | CONFLICT | UNP G1TM82 |
| VV    | 75      | ALA      | SER    | CONFLICT | UNP G1TM82 |

- Molecule 74 is a protein called uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | WW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 75 is a protein called uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | XX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 76 is a protein called eS24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | YY    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 646 | 200 | 172 | 5 |         |       |

- Molecule 77 is a protein called eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | ZZ    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 78 is a protein called eS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | aa    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 486 | 161 | 129 | 5 |         |       |

- Molecule 79 is a protein called eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | bb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 80 is a protein called eS28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | cc    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 475   | 290 | 92 | 91 | 2 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| cc    | 18      | ILE      | LEU    | CONFLICT | UNP G1TIB4 |
| cc    | 20      | LYS      | ARG    | CONFLICT | UNP G1TIB4 |
| cc    | 40      | HIS      | ARG    | CONFLICT | UNP G1TIB4 |
| cc    | 42      | THR      | ILE    | CONFLICT | UNP G1TIB4 |

- Molecule 81 is a protein called uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 81  | dd    | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 445   | 278 | 90 | 72 | 5 |         |       |

- Molecule 82 is a protein called eS30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 82  | ee    | 57       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 457   | 282 | 101 | 73 | 1 |         |       |

- Molecule 83 is a protein called eS31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 83  | ff    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 520   | 331 | 98 | 85 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| ff    | ?       | -        | VAL    | DELETION | UNP G1SK22 |

- Molecule 84 is a protein called RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 84  | gg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 85 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 85  | hh    | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 257   | 115 | 46 | 84 | 12 |         |       |

- Molecule 86 is a protein called eRF1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 86  | ii    | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2087 | 559 | 623 | 11 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| ii    | 183     | ALA      | GLY    | ENGINEERED MUTATION | UNP P62495 |
| ii    | 184     | ALA      | GLY    | ENGINEERED MUTATION | UNP P62495 |

- Molecule 87 is a protein called ABCE1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 87  | jj    | 576      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4543  | 2904 | 779 | 829 | 31 |         |       |

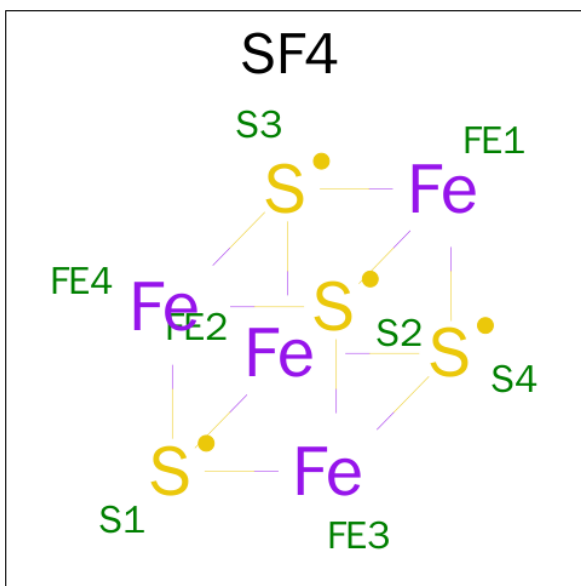
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 88  | P     | 1        | Total Mg<br>1 1     | 0       |
| 88  | g     | 1        | Total Mg<br>1 1     | 0       |
| 88  | LL    | 1        | Total Mg<br>1 1     | 0       |
| 88  | B     | 1        | Total Mg<br>1 1     | 0       |
| 88  | I     | 1        | Total Mg<br>1 1     | 0       |
| 88  | C     | 1        | Total Mg<br>1 1     | 0       |
| 88  | V     | 1        | Total Mg<br>1 1     | 0       |
| 88  | 7     | 5        | Total Mg<br>5 5     | 0       |
| 88  | 5     | 146      | Total Mg<br>146 146 | 0       |
| 88  | 8     | 2        | Total Mg<br>2 2     | 0       |
| 88  | 9     | 34       | Total Mg<br>34 34   | 0       |
| 88  | hh    | 1        | Total Mg<br>1 1     | 0       |

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

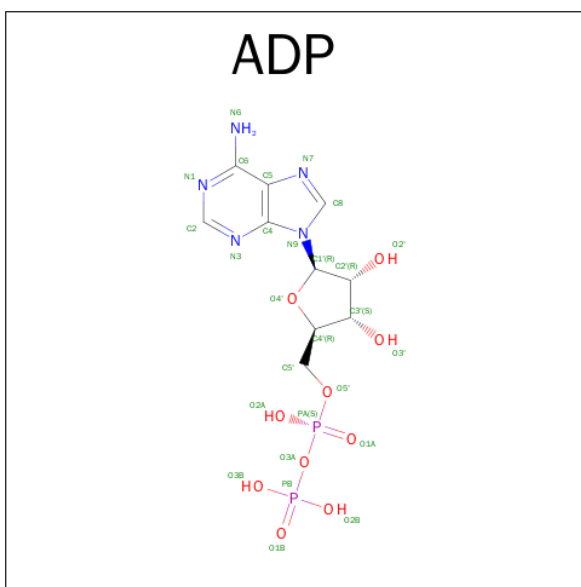
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 89  | p     | 1        | Total Zn<br>1 1 | 0       |
| 89  | g     | 1        | Total Zn<br>1 1 | 0       |
| 89  | j     | 1        | Total Zn<br>1 1 | 0       |
| 89  | dd    | 1        | Total Zn<br>1 1 | 0       |
| 89  | ff    | 1        | Total Zn<br>1 1 | 0       |
| 89  | aa    | 1        | Total Zn<br>1 1 | 0       |
| 89  | o     | 1        | Total Zn<br>1 1 | 0       |
| 89  | m     | 1        | Total Zn<br>1 1 | 0       |

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 90  | jj    | 1        | Total | Fe | S | 0       |
|     |       |          | 16    | 8  | 8 |         |
| 90  | jj    | 1        | Total | Fe | S | 0       |
|     |       |          | 16    | 8  | 8 |         |

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).

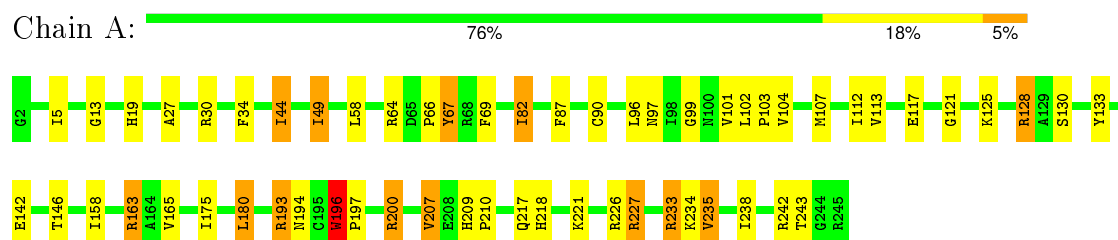


| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|
| 91  | jj    | 1        | Total | C  | N  | O  | P | 0       |
|     |       |          | 54    | 20 | 10 | 20 | 4 |         |
| 91  | jj    | 1        | Total | C  | N  | O  | P | 0       |
|     |       |          | 54    | 20 | 10 | 20 | 4 |         |

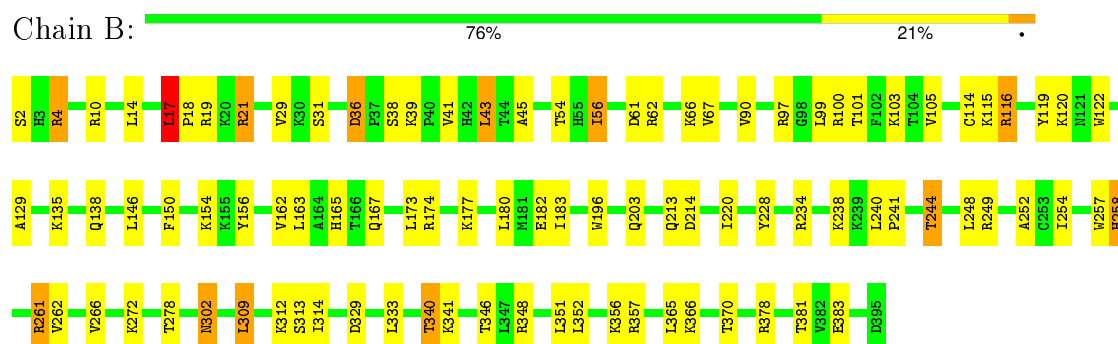
### 3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

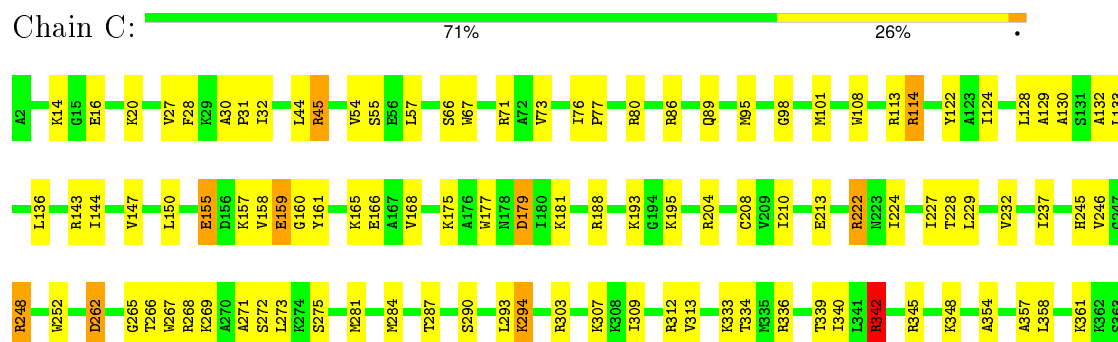
#### • Molecule 1: uL2



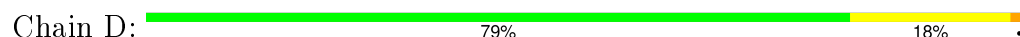
#### • Molecule 2: uL3



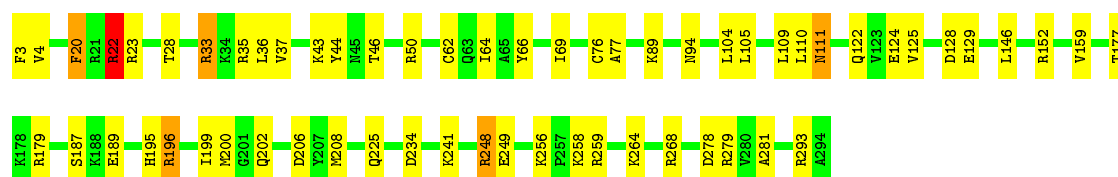
#### • Molecule 3: uL4



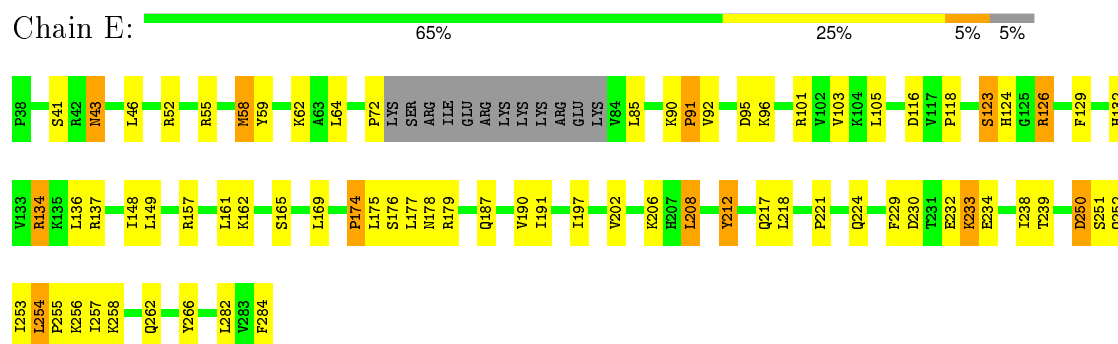
#### • Molecule 4: uL18



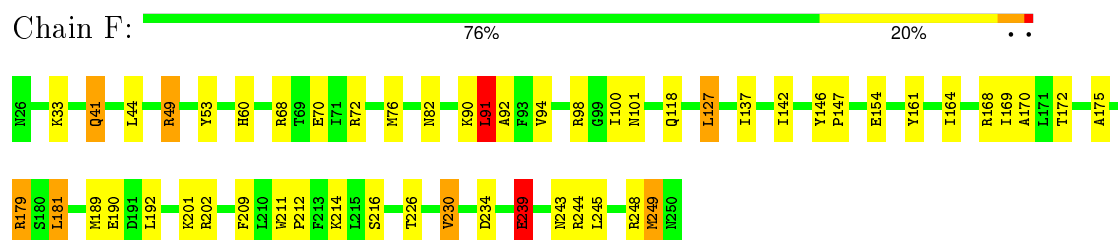




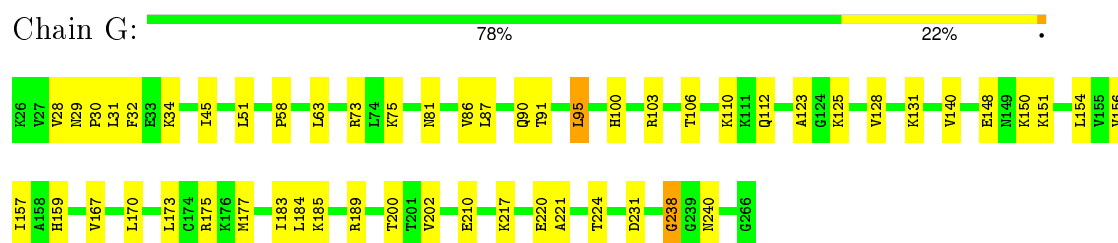
- Molecule 5: eL6



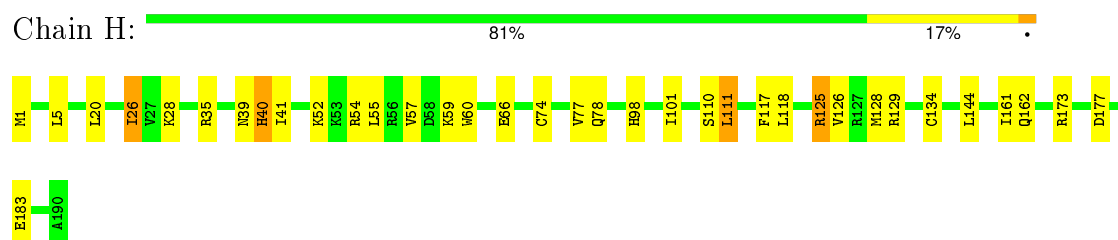
- Molecule 6: uL30



- Molecule 7: eL8

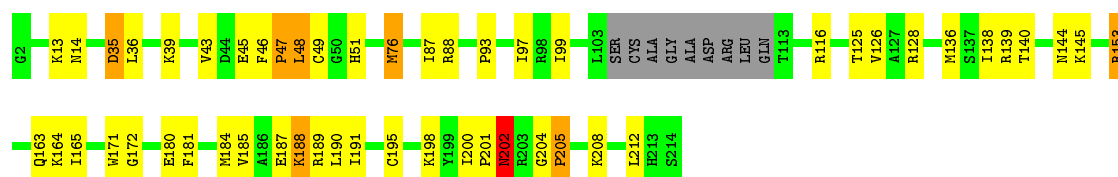


- Molecule 8: uL6



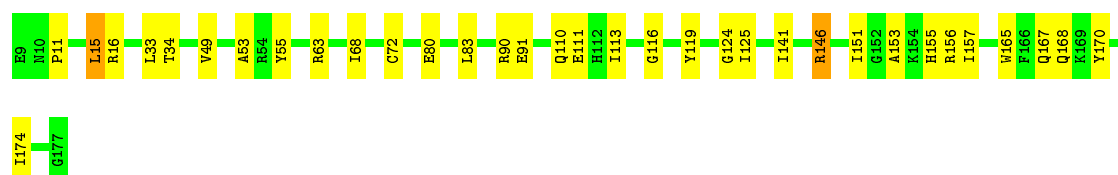
- Molecule 9: uL16





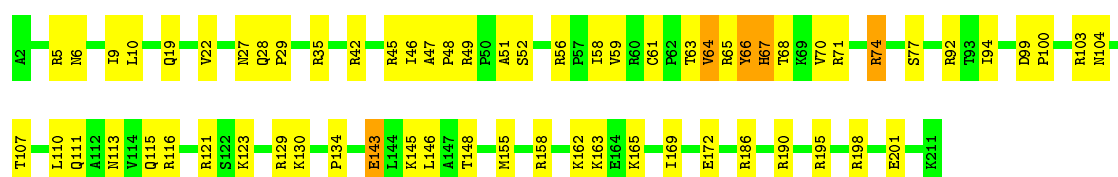
• Molecule 10: uL5

Chain J: 80% 19%



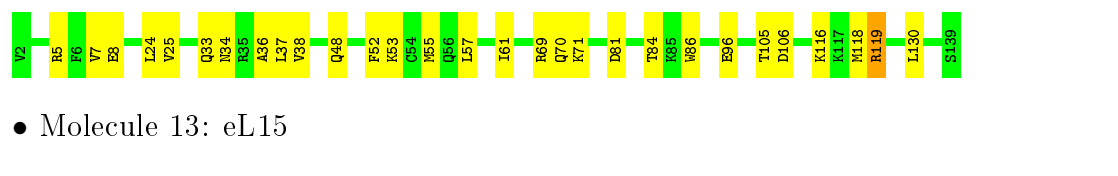
• Molecule 11: eL13

Chain L: 69% 29%



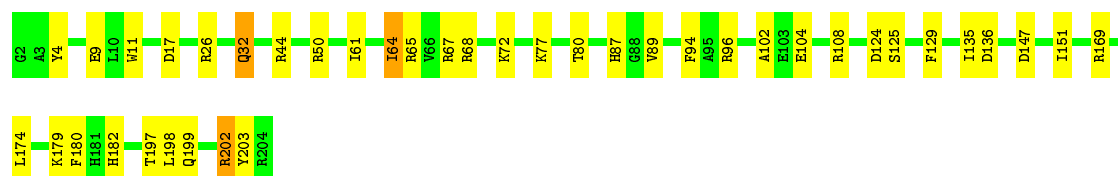
• Molecule 12: eL14

Chain M: 79% 20%



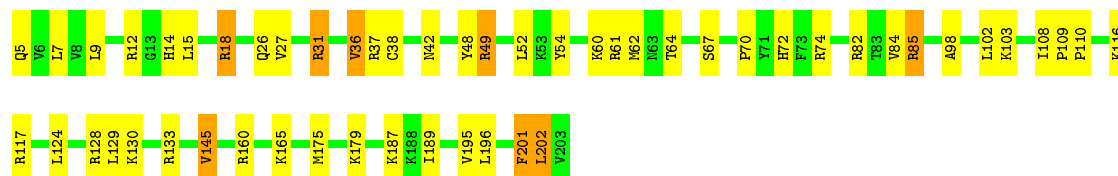
• Molecule 13: eL15

Chain N: 80% 18%




• Molecule 14: uL13

Chain O: 73% 23%




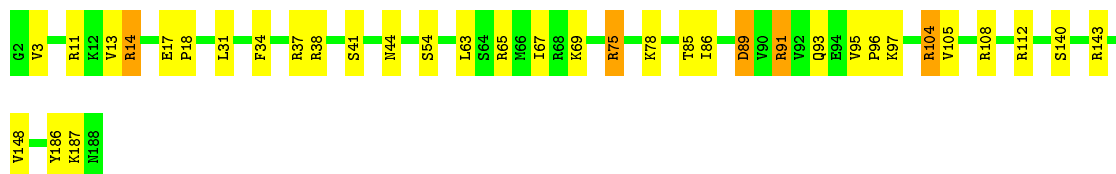
- Molecule 15: uL22

Chain P:  84% 14%



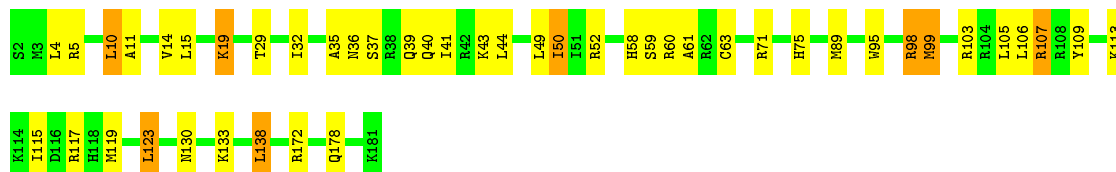
- Molecule 16: uL14

Chain Q:  81% 17%




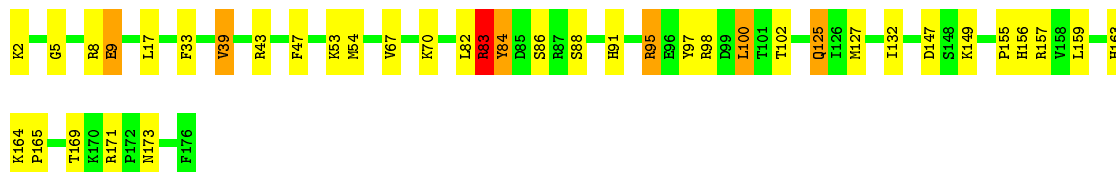
- Molecule 17: eL19

Chain R:  74% 21%




- Molecule 18: eL20

Chain S:  78% 18%




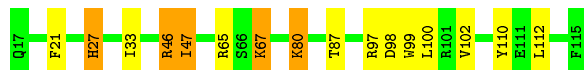
- Molecule 19: eL21

Chain T:  80% 19%




- Molecule 20: eL22

Chain U:  84% 11% 5%




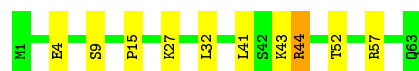
- Molecule 21: uL14

Chain V:  81% 18%




- Molecule 22: eL24

Chain W:  84% 14%




- Molecule 23: uL23

Chain X:  82% 16%



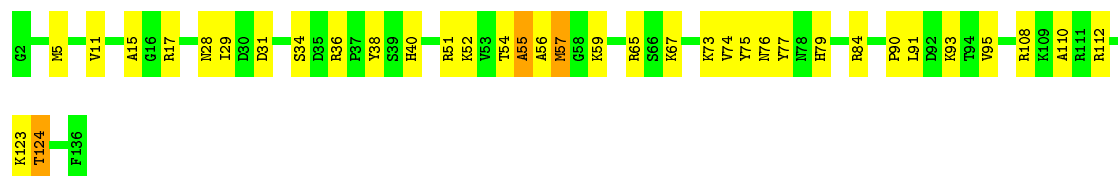
- Molecule 24: uL24

Chain Y:  81% 14%




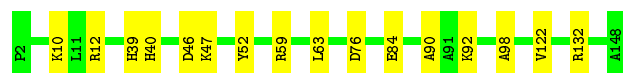
- Molecule 25: eL27

Chain Z:  73% 24%



- Molecule 26: uL15

Chain a:  89% 11%




- Molecule 27: eL29

Chain b:  92% 8%




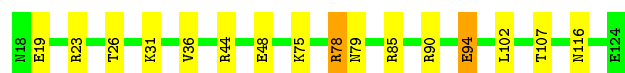
- Molecule 28: eL30

Chain c:  86% 14%




- Molecule 29: eL31

Chain d:  85% 13%




- Molecule 30: eL32

Chain e:  84% 16%




- Molecule 31: eL33

Chain f:  83% 17%




- Molecule 32: eL34

Chain g:  86% 13%




- Molecule 33: uL29

Chain h:  88% 11%




- Molecule 34: eL36

Chain i:  91% 9%

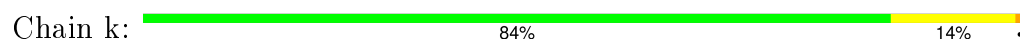


- Molecule 35: eL37

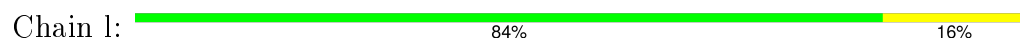
Chain j:  83% 15%



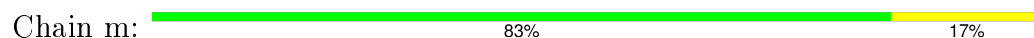
- Molecule 36: eL38



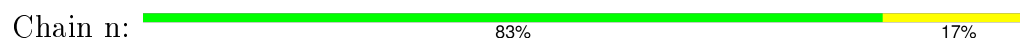
- Molecule 37: eL39



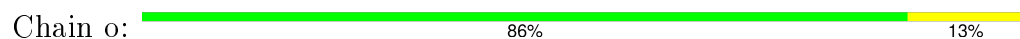
- Molecule 38: eL40



- Molecule 39: eL41



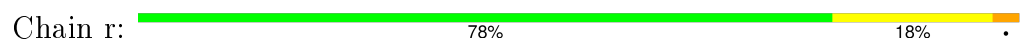
- Molecule 40: eL42



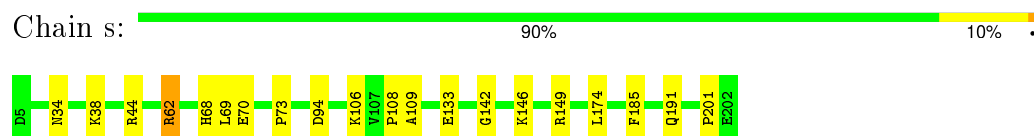
- Molecule 41: eL43



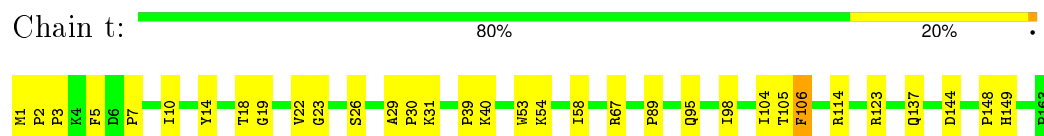
- Molecule 42: eL28



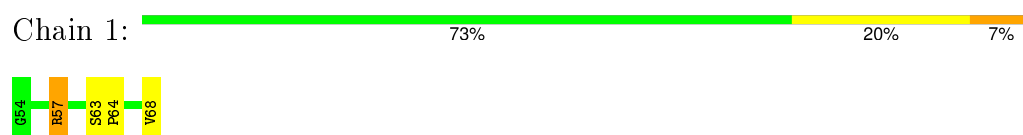
- Molecule 43: uL10



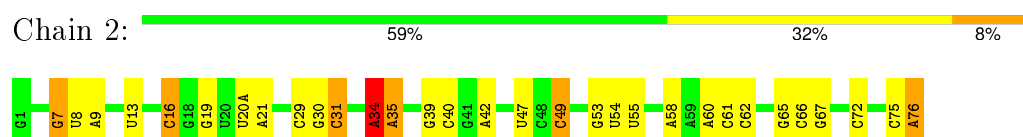
- Molecule 44: uL11



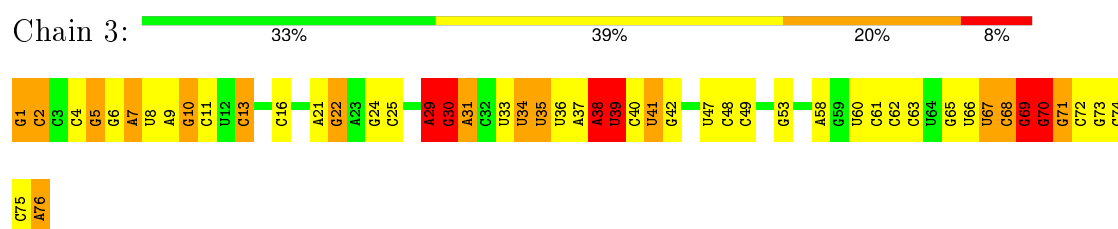
- Molecule 45: peptide



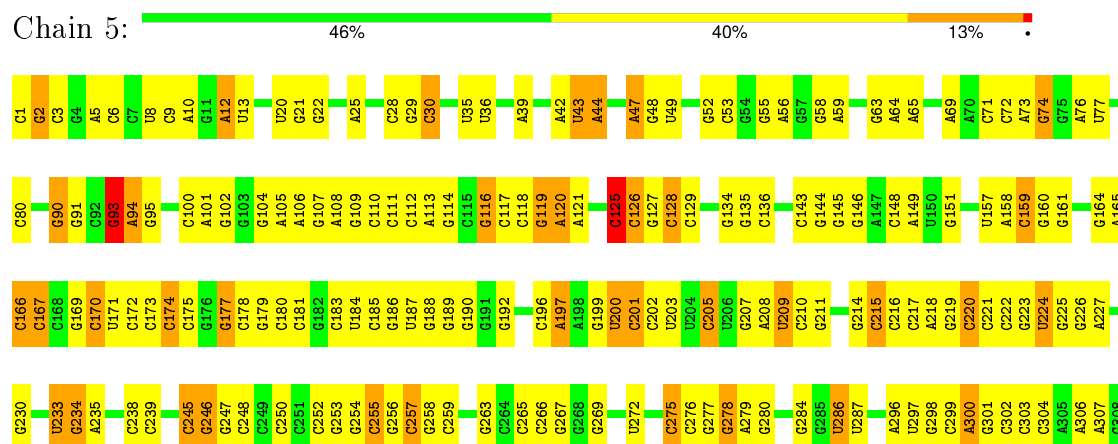
- Molecule 46: tRNA(Val)



- Molecule 47: tRNA(Lys)



- Molecule 48: 28S ribosomal RNA



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
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| C1963 | C1964 | C1965 | C1966 | C1967 | C1968 | C1969 | C1970 | C1971 | C1972 | C1973 | C1974 | C1975 | C1976 | C1977 | C1978 | C1979 | C1980 | C1981 | C1982 | C1983 | C1984 | C1985 | C1986 | C1987 | C1988 | C1989 | C1990 | C1991 | C1992 | C1993 | C1994 | C1995 | C1996 | C1997 | C1998 | C1999 | C2000 | C2001 | C2002 | C2003 | C2004 | C2005 | C2006 | C2007 | C2008 | C2009 | C2010 | C2011 | C2012 | C2013 | C2014 | C2015 | C2016 | C2017 | C2018 | C2019 | C2020 | C2021 | C2022 | C2023 | C2024 | C2025 | C2026 | C2027 | C2028 | C2029 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A1787 | A1788 | A1789 | A1790 | A1791 | A1792 | A1793 | A1794 | A1795 | A1796 | A1797 | A1798 | A1799 | A1800 | A1801 | A1802 | A1803 | A1804 | A1805 | A1806 | A1807 | A1808 | A1809 | A1810 | A1811 | A1812 | A1813 | A1814 | A1815 | A1816 | A1817 | A1818 | A1819 | A1820 | A1821 | A1822 | A1823 | A1824 | A1825 | A1826 | A1827 | A1828 | A1829 | A1830 | A1831 | A1832 | A1833 | A1834 | A1835 | A1836 | A1837 | A1838 | A1839 | A1840 | A1841 | A1842 | A1843 | A1844 | A1845 | A1846 | A1847 | A1848 | A1849 | A1850 | A1851 | A1852 | A1853 | A1854 | A1855 | A1856 | A1857 | A1858 | A1859 | A1860 | A1861 | A1862 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G1589 | G1590 | G1591 | G1592 | G1593 | G1594 | G1595 | G1596 | G1597 | G1598 | G1599 | G1600 | G1601 | G1602 | G1603 | G1604 | G1605 | G1606 | G1607 | G1608 | G1609 | G1610 | G1611 | G1612 | G1613 | G1614 | G1615 | G1616 | G1617 | G1618 | G1619 | G1620 | G1621 | G1622 | G1623 | G1624 | G1625 | G1626 | G1627 | G1628 | G1629 | G1630 | G1631 | G1632 | G1633 | G1634 | G1635 | G1636 | G1637 | G1638 | G1639 | G1640 | G1641 | G1642 | G1643 | G1644 | G1645 | G1646 | G1647 | G1648 | G1649 | G1650 | G1651 | G1652 | G1653 | G1654 | G1655 | G1656 | G1657 | G1658 | G1659 | G1660 | G1661 | G1662 | G1663 | G1664 | G1665 | G1666 | G1667 | G1668 | G1669 | G1670 | G1671 | G1672 | G1673 | G1674 | G1675 | G1676 | G1677 | G1678 | G1679 | G1680 | G1681 | G1682 | G1683 | G1684 | G1685 | G1686 | G1687 | G1688 | G1689 | G1690 | G1691 | G1692 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C1414 | C1415 | C1416 | C1417 | C1418 | C1419 | C1420 | C1421 | C1422 | C1423 | C1424 | C1425 | C1426 | C1427 | C1428 | C1429 | C1430 | C1431 | C1432 | C1433 | C1434 | C1435 | C1436 | C1437 | C1438 | C1439 | C1440 | C1441 | C1442 | C1443 | C1444 | C1445 | C1446 | C1447 | C1448 | C1449 | C1450 | C1451 | C1452 | C1453 | C1454 | C1455 | C1456 | C1457 | C1458 | C1459 | C1460 | C1461 | C1462 | C1463 | C1464 | C1465 | C1466 | C1467 | C1468 | C1469 | C1470 | C1471 | C1472 | C1473 | C1474 | C1475 | C1476 | C1477 | C1478 | C1479 | C1480 | C1481 | C1482 | C1483 | C1484 | C1485 | C1486 | C1487 | C1488 | C1489 | C1490 | C1491 | C1492 | C1493 | C1494 | C1495 | C1496 | C1497 | C1498 | C1499 | C1500 | C1501 | C1502 | C1503 | C1504 | C1505 | C1506 | C1507 | C1508 | C1509 | C1510 | C1511 | C1512 | C1513 | C1514 | C1515 | C1516 | C1517 | C1518 | C1519 | C1520 | C1521 | C1522 | C1523 | C1524 | C1525 | C1526 | C1527 | C1528 | C1529 | C1530 | C1531 | C1532 | C1533 | C1534 | C1535 | C1536 | C1537 | C1538 | C1539 | C1540 | C1541 | C1542 | C1543 | C1544 | C1545 | C1546 | C1547 | C1548 | C1549 | C1550 | C1551 | C1552 | C1553 | C1554 | C1555 | C1556 | C1557 | C1558 | C1559 | C1560 | C1561 | C1562 | C1563 | C1564 | C1565 | C1566 | C1567 | C1568 | C1569 | C1570 | C1571 | C1572 | C1573 | C1574 | C1575 | C1576 | C1577 | C1578 | C1579 | C1580 | C1581 | C1582 | C1583 | C1584 | C1585 | C1586 | C1587 | C1588 | C1589 | C1590 | C1591 | C1592 | C1593 | C1594 | C1595 | C1596 | C1597 | C1598 | C1599 | C1600 | C1601 | C1602 | C1603 | C1604 | C1605 | C1606 | C1607 | C1608 | C1609 | C1610 | C1611 | C1612 | C1613 | C1614 | C1615 | C1616 | C1617 | C1618 | C1619 | C1620 | C1621 | C1622 | C1623 | C1624 | C1625 | C1626 | C1627 | C1628 | C1629 | C1630 | C1631 | C1632 | C1633 | C1634 | C1635 | C1636 | C1637 | C1638 | C1639 | C1640 | C1641 | C1642 | C1643 | C1644 | C1645 | C1646 | C1647 | C1648 | C1649 | C1650 | C1651 | C1652 | C1653 | C1654 | C1655 | C1656 | C1657 | C1658 | C1659 | C1660 | C1661 | C1662 | C1663 | C1664 | C1665 | C1666 | C1667 | C1668 | C1669 | C1670 | C1671 | C1672 | C1673 | C1674 | C1675 | C1676 | C1677 | C1678 | C1679 | C1680 | C1681 | C1682 | C1683 | C1684 | C1685 | C1686 | C1687 | C1688 | C1689 | C1690 | C1691 | C1692 | C1693 | C1694 | C1695 | C1696 | C1697 | C1698 | C1699 | C1700 | C1701 | C1702 | C1703 | C1704 | C1705 | C1706 | C1707 | C1708 | C1709 | C1710 | C1711 | C1712 | C1713 | C1714 | C1715 | C1716 | C1717 | C1718 | C1719 | C1720 | C1721 | C1722 | C1723 | C1724 | C1725 | C1726 | C1727 | C1728 | C1729 | C1730 | C1731 | C1732 | C1733 | C1734 | C1735 | C1736 | C1737 | C1738 | C1739 | C1740 | C1741 | C1742 | C1743 | C1744 | C1745 | C1746 | C1747 | C1748 | C1749 | C1750 | C1751 | C1752 | C1753 | C1754 | C1755 | C1756 | C1757 | C1758 | C1759 | C1760 | C1761 | C1762 | C1763 | C1764 | C1765 | C1766 | C1767 | C1768 | C1769 | C1770 | C1771 | C1772 | C1773 | C1774 | C1775 | C1776 | C1777 | C1778 | C1779 | C1780 | C1781 | C1782 | C1783 | C1784 | C1785 | C1786 | C1787 | C1788 | C1789 | C1790 | C1791 | C1792 | C1793 | C1794 | C1795 | C1796 | C1797 | C1798 | C1799 | C1800 | C1801 | C1802 | C1803 | C1804 | C1805 | C1806 | C1807 | C1808 | C1809 | C1810 | C1811 | C1812 | C1813 | C1814 | C1815 | C1816 | C1817 | C1818 | C1819 | C1820 | C1821 | C1822 | C1823 | C1824 | C1825 | C1826 | C1827 | C1828 | C1829 | C1830 | C1831 | C1832 | C1833 | C1834 | C1835 | C1836 | C1837 | C1838 | C1839 | C1840 | C1841 | C1842 | C1843 | C1844 | C1845 | C1846 | C1847 | C1848 | C1849 | C1850 | C1851 | C1852 | C1853 | C1854 | C1855 | C1856 | C1857 | C1858 | C1859 | C1860 | C1861 | C1862 | C1863 | C1864 | C1865 | C1866 | C1867 | C1868 | C1869 | C1870 | C1871 | C1872 | C1873 | C1874 | C1875 | C1876 | C1877 | C1878 | C1879 | C1880 | C1881 | C1882 | C1883 | C1884 | C1885 | C1886 | C1887 | C1888 | C1889 | C1890 | C1891 | C1892 | C1893 | C1894 | C1895 | C1896 | C1897 | C1898 | C1899 | C1900 | C1901 | C1902 | C1903 | C1904 | C1905 | C1906 | C1907 | C1908 | C1909 | C1910 | C1911 | C1912 | C1913 | C1914 | C1915 | C1916 | C1917 | C1918 | C1919 | C1920 | C1921 | C1922 | C1923 | C1924 | C1925 | C1926 | C1927 | C1928 | C1929 | C1930 | C1931 | C1932 | C1933 | C1934 | C1935 | C1936 | C1937 | C1938 | C1939 | C1940 | C1941 | C1942 | C1943 | C1944 | C1945 | C1946 | C1947 | C1948 | C1949 | C1950 | C1951 | C1952 | C1953 | C1954 | C1955 | C1956 | C1957 | C1958 | C1959 | C1960 | C1961 | C1962 | C1963 | C1964 | C1965 | C1966 | C1967 | C1968 | C1969 | C1970 | C1971 | C1972 | C1973 | C1974 | C1975 | C1976 | C1977 | C1978 | C1979 | C1980 | C1981 | C1982 | C1983 | C1984 | C1985 | C1986 | C1987 | C1988 | C1989 | C1990 | C1991 | C1992 | C1993 | C1994 | C1995 | C1996 | C1997 | C1998 | C1999 | C2000 | C2001 | C2002 | C2003 | C2004 | C2005 | C2006 | C2007 | C2008 | C2009 | C2010 | C2011 | C2012 | C2013 | C2014 | C2015 | C2016 | C2017 | C2018 | C2019 | C2020 | C2021 | C2022 | C2023 | C2024 | C2025 | C2026 | C2027 | C2028 | C2029 |
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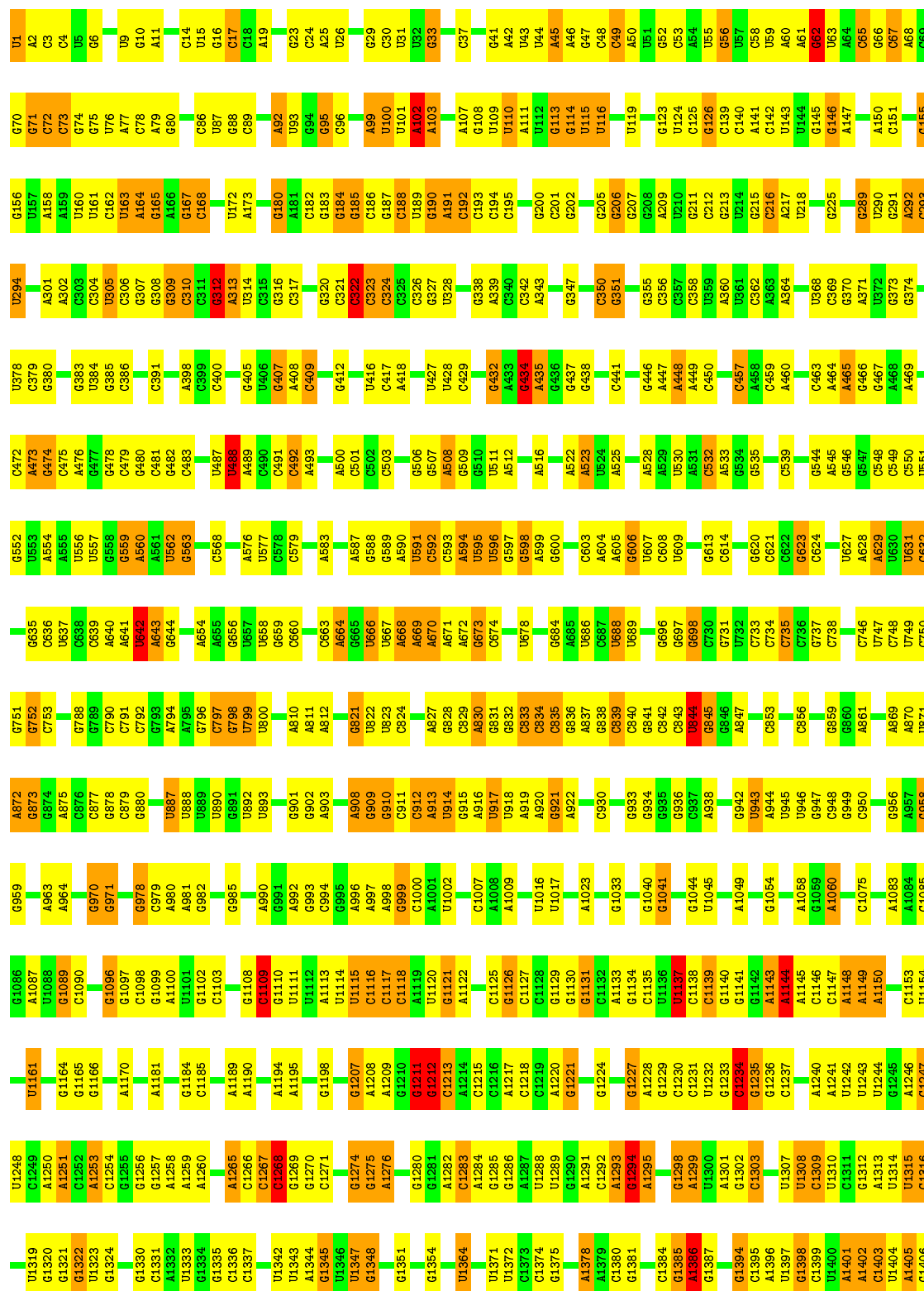


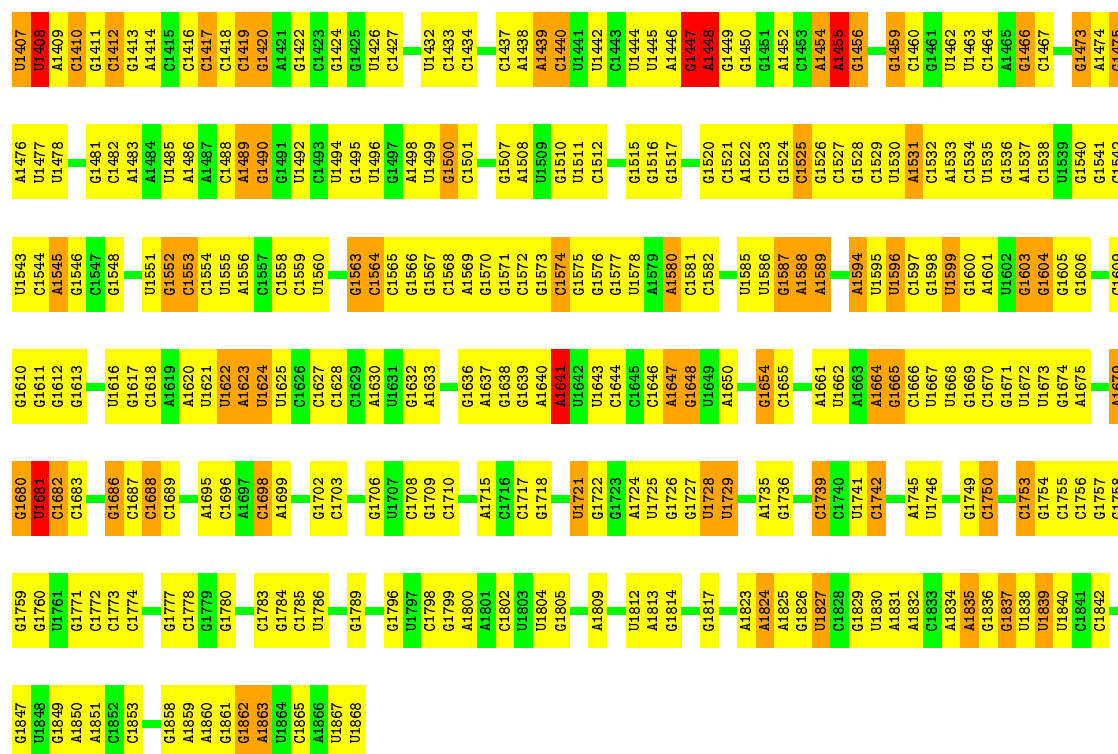
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|       |       |       | G3794 | G3814 | C3620 | G2842 | U2752 | G2586 | A2432 | U2413 |       |       |
|       |       |       | G3795 | G3815 | C3621 | G2843 | U2753 | G2587 | A2433 | U2414 |       |       |
|       |       |       | G3796 | G3816 | C3622 | G2844 | U2754 | G2588 | A2434 | U2415 |       |       |
|       |       |       | G3797 | G3817 | C3623 | G2845 | U2755 | G2589 | A2435 | U2416 |       |       |
|       |       |       | G3798 | G3818 | C3624 | G2846 | U2756 | G2590 | A2436 | U2417 |       |       |
|       |       |       | G3799 | G3819 | C3625 | G2847 | U2757 | G2591 | A2437 | U2418 |       |       |
|       |       |       | G3800 | G3820 | C3626 | G2848 | U2758 | G2592 | A2438 | U2419 |       |       |
|       |       |       | G3801 | G3821 | C3627 | G2849 | U2759 | G2593 | A2439 | U2420 |       |       |
|       |       |       | G3802 | G3822 | C3628 | G2850 | U2760 | G2594 | A2440 | U2421 |       |       |
|       |       |       | G3803 | G3823 | C3629 | G2851 | U2761 | G2595 | A2441 | U2422 |       |       |
|       |       |       | G3804 | G3824 | C3630 | G2852 | U2762 | G2596 | A2442 | U2423 |       |       |
|       |       |       | G3805 | G3825 | C3631 | G2853 | U2763 | G2597 | A2443 | U2424 |       |       |
|       |       |       | G3806 | G3826 | C3632 | G2854 | U2764 | G2598 | A2444 | U2425 |       |       |
|       |       |       | G3807 | G3827 | C3633 | G2855 | U2765 | G2599 | A2445 | U2426 |       |       |
|       |       |       | G3808 | G3828 | C3634 | G2856 | U2766 | G2600 | A2446 | U2427 |       |       |
|       |       |       | G3809 | G3829 | C3635 | G2857 | U2767 | G2601 | A2447 | U2428 |       |       |
|       |       |       | G3810 | G3830 | C3636 | G2858 | U2768 | G2602 | A2448 | U2429 |       |       |
|       |       |       | G3811 | G3831 | C3637 | G2859 | U2769 | G2603 | A2449 | U2430 |       |       |
|       |       |       | G3812 | G3832 | C3638 | G2860 | U2770 | G2604 | A2450 | U2431 |       |       |
|       |       |       | G3813 | G3833 | C3639 | G2861 | U2771 | G2605 | A2451 | U2432 |       |       |
|       |       |       | G3814 | G3834 | C3640 | G2862 | U2772 | G2606 | A2452 | U2433 |       |       |
|       |       |       | G3815 | G3835 | C3641 | G2863 | U2773 | G2607 | A2453 | U2434 |       |       |
|       |       |       | G3816 | G3836 | C3642 | G2864 | U2774 | G2608 | A2454 | U2435 |       |       |
|       |       |       | G3817 | G3837 | C3643 | G2865 | U2775 | G2609 | A2455 | U2436 |       |       |
|       |       |       | G3818 | G3838 | C3644 | G2866 | U2776 | G2610 | A2456 | U2437 |       |       |
|       |       |       | G3819 | G3839 | C3645 | G2867 | U2777 | G2611 | A2457 | U2438 |       |       |
|       |       |       | G3820 | G3840 | C3646 | G2868 | U2778 | G2612 | A2458 | U2439 |       |       |
|       |       |       | G3821 | G3841 | C3647 | G2869 | U2779 | G2613 | A2459 | U2440 |       |       |
|       |       |       | G3822 | G3842 | C3648 | G2870 | U2780 | G2614 | A2460 | U2441 |       |       |
|       |       |       | G3823 | G3843 | C3649 | G2871 | U2781 | G2615 | A2461 | U2442 |       |       |
|       |       |       | G3824 | G3844 | C3650 | G2872 | U2782 | G2616 | A2462 | U2443 |       |       |
|       |       |       | G3825 | G3845 | C3651 | G2873 | U2783 | G2617 | A2463 | U2444 |       |       |
|       |       |       | G3826 | G3846 | C3652 | G2874 | U2784 | G2618 | A2464 | U2445 |       |       |
|       |       |       | G3827 | G3847 | C3653 | G2875 | U2785 | G2619 | A2465 | U2446 |       |       |
|       |       |       | G3828 | G3848 | C3654 | G2876 | U2786 | G2620 | A2466 | U2447 |       |       |
|       |       |       | G3829 | G3849 | C3655 | G2877 | U2787 | G2621 | A2467 | U2448 |       |       |
|       |       |       | G3830 | G3850 | C3656 | G2878 | U2788 | G2622 | A2468 | U2449 |       |       |
|       |       |       | G3831 | G3851 | C3657 | G2879 | U2789 | G2623 | A2469 | U2450 |       |       |
|       |       |       | G3832 | G3852 | C3658 | G2880 | U2790 | G2624 | A2470 | U2451 |       |       |
|       |       |       | G3833 | G3853 | C3659 | G2881 | U2791 | G2625 | A2471 | U2452 |       |       |
|       |       |       | G3834 | G3854 | C3660 | G2882 | U2792 | G2626 | A2472 | U2453 |       |       |
|       |       |       | G3835 | G3855 | C3661 | G2883 | U2793 | G2627 | A2473 | U2454 |       |       |
|       |       |       | G3836 | G3856 | C3662 | G2884 | U2794 | G2628 | A2474 | U2455 |       |       |
|       |       |       | G3837 | G3857 | C3663 | G2885 | U2795 | G2629 | A2475 | U2456 |       |       |
|       |       |       | G3838 | G3858 | C3664 | G2886 | U2796 | G2630 | A2476 | U2457 |       |       |
|       |       |       | G3839 | G3859 | C3665 | G2887 | U2797 | G2631 | A2477 | U2458 |       |       |
|       |       |       | G3840 | G3860 | C3666 | G2888 | U2798 | G2632 | A2478 | U2459 |       |       |
|       |       |       | G3841 | G3861 | C3667 | G2889 | U2799 | G2633 | A2479 | U2460 |       |       |
|       |       |       | G3842 | G3862 | C3668 | G2890 | U2800 | G2634 | A2480 | U2461 |       |       |
|       |       |       | G3843 | G3863 | C3669 | G2891 | U2801 | G2635 | A2481 | U2462 |       |       |
|       |       |       | G3844 | G3864 | C3670 | G2892 | U2802 | G2636 | A2482 | U2463 |       |       |
|       |       |       | G3845 | G3865 | C3671 | G2893 | U2803 | G2637 | A2483 | U2464 |       |       |
|       |       |       | G3846 | G3866 | C3672 | G2894 | U2804 | G2638 | A2484 | U2465 |       |       |
|       |       |       | G3847 | G3867 | C3673 | G2895 | U2805 | G2639 | A2485 | U2466 |       |       |
|       |       |       | G3848 | G3868 | C3674 | G2896 | U2806 | G2640 | A2486 | U2467 |       |       |
|       |       |       | G3849 | G3869 | C3675 | G2897 | U2807 | G2641 | A2487 | U2468 |       |       |
|       |       |       | G3850 | G3870 | C3676 | G2898 | U2808 | G2642 | A2488 | U2469 |       |       |
|       |       |       | G3851 | G3871 | C3677 | G2899 | U2809 | G2643 | A2489 | U2470 |       |       |
|       |       |       | G3852 | G3872 | C3678 | G2900 | U2810 | G2644 | A2490 | U2471 |       |       |
|       |       |       | G3853 | G3873 | C3679 | G2901 | U2811 | G2645 | A2491 | U2472 |       |       |
|       |       |       | G3854 | G3874 | C3680 | G2902 | U2812 | G2646 | A2492 | U2473 |       |       |
|       |       |       | G3855 | G3875 | C3681 | G2903 | U2813 | G2647 | A2493 | U2474 |       |       |
|       |       |       | G3856 | G3876 | C3682 | G2904 | U2814 | G2648 | A2494 | U2475 |       |       |
|       |       |       | G3857 | G3877 | C3683 | G2905 | U2815 | G2649 | A2495 | U2476 |       |       |
|       |       |       | G3858 | G3878 | C3684 | G2906 | U2816 | G2650 | A2496 | U2477 |       |       |
|       |       |       | G3859 | G3879 | C3685 | G2907 | U2817 | G2651 | A2497 | U2478 |       |       |
|       |       |       | G3860 | G3880 | C3686 | G2908 | U2818 | G2652 | A2498 | U2479 |       |       |
|       |       |       | G3861 | G3881 | C3687 | G2909 | U2819 | G2653 | A2499 | U2480 |       |       |
|       |       |       | G3862 | G3882 | C3688 | G2910 | U2820 | G2654 | A2500 | U2481 |       |       |
|       |       |       | G3863 | G3883 | C3689 | G2911 | U2821 | G2655 | A2501 | U2482 |       |       |
|       |       |       | G3864 | G3884 | C3690 | G2912 | U2822 | G2656 | A2502 | U2483 |       |       |
|       |       |       | G3865 | G3885 | C3691 | G2913 | U2823 | G2657 | A2503 | U2484 |       |       |
|       |       |       | G3866 | G3886 | C3692 | G2914 | U2824 | G2658 | A2504 | U2485 |       |       |
|       |       |       | G3867 | G3887 | C3693 | G2915 | U2825 | G2659 | A2505 | U2486 |       |       |
|       |       |       | G3868 | G3888 | C3694 | G2916 | U2826 | G2660 | A2506 | U2487 |       |       |
|       |       |       | G3869 | G3889 | C3695 | G2917 | U2827 | G2661 | A2507 | U2488 |       |       |
|       |       |       | G3870 | G3890 | C3696 | G2918 | U2828 | G2662 | A2508 | U2489 |       |       |
|       |       |       | G3871 | G3891 | C3697 | G2919 | U2829 | G2663 | A2509 | U2490 |       |       |
|       |       |       | G3872 | G3892 | C3698 | G2920 | U2830 | G2664 | A2510 | U2491 |       |       |
|       |       |       | G3873 | G3893 | C3699 | G2921 | U2831 | G2665 | A2511 | U2492 |       |       |
|       |       |       | G3874 | G3894 | C3700 | G2922 | U2832 | G2666 | A2512 | U2493 |       |       |
|       |       |       | G3875 | G3895 | C3701 | G2923 | U2833 | G2667 | A2513 | U2494 |       |       |
|       |       |       | G3876 | G3896 | C3702 | G2924 | U2834 | G2668 | A2514 | U2495 |       |       |
|       |       |       | G3877 | G3897 | C3703 | G2925 | U2835 | G2669 | A2515 | U2496 |       |       |
|       |       |       | G3878 | G3898 | C3704 | G2926 | U2836 | G2670 | A2516 | U2497 |       |       |
|       |       |       | G3879 | G3899 | C3705 | G2927 | U2837 | G2671 | A2517 | U2498 |       |       |
|       |       |       | G3880 | G3900 | C3706 | G2928 | U2838 | G2672 | A2518 | U2499 |       |       |
|       |       |       | G3881 | G3901 | C3707 | G2929 | U2839 | G2673 | A2519 | U2500 |       |       |
|       |       |       | G3882 | G3902 | C3708 | G2930 | U2840 | G2674 | A2520 | U2501 |       |       |
|       |       |       | G3883 | G3903 | C3709 | G2931 | U2841 | G2675 | A2521 | U2502 |       |       |
|       |       |       | G3884 | G3904 | C3710 | G2932 | U2842 | G2676 | A2522 | U2503 |       |       |
|       |       |       | G3885 | G3905 | C3711 | G2933 | U2843 | G2677 | A2523 | U2504 |       |       |
|       |       |       | G3886 | G3906 | C3712 | G2934 | U2844 | G2678 | A2524 | U2505 |       |       |
|       |       |       | G3887 | G3907 | C3713 | G2935 | U2845 | G2679 | A2525 | U2506 |       |       |



• Molecule 51: 18S ribosomal RNA

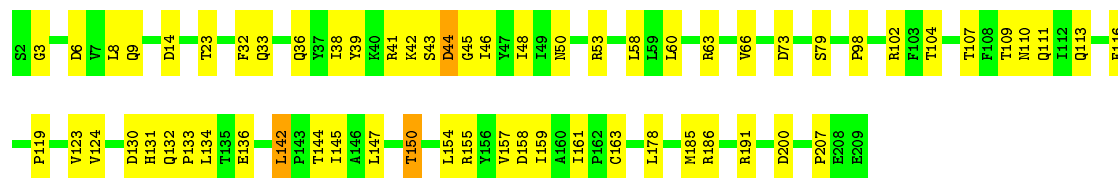
Chain 9: 





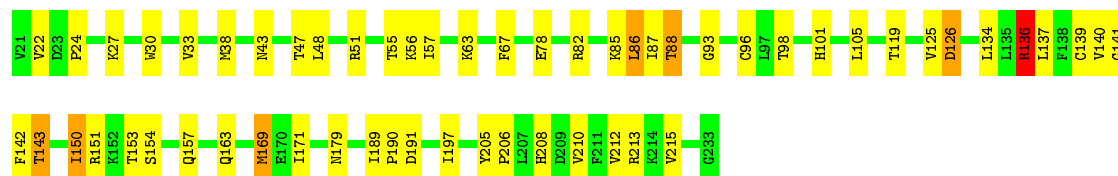
• Molecule 52: uS2

Chain AA: 70% 28%



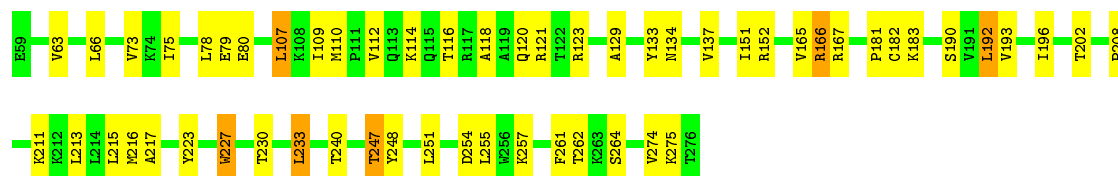
• Molecule 53: eS1

Chain BB: 73% 23%




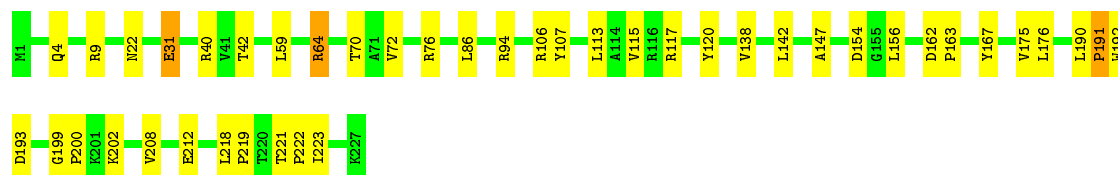
• Molecule 54: uS5

Chain CC: 74% 23%



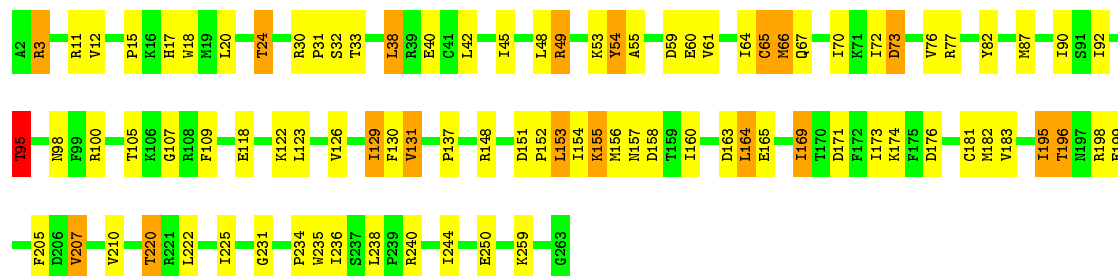
- Molecule 55: uS3

Chain DD: 



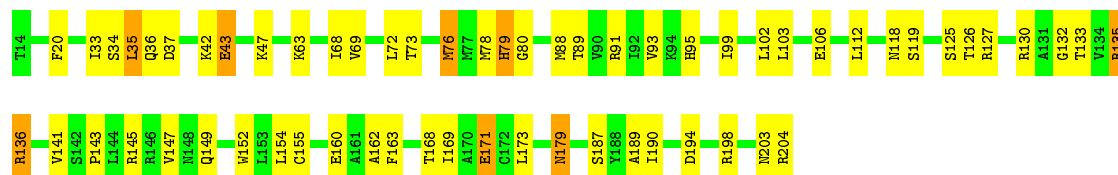
- Molecule 56: eS4

Chain EE: 




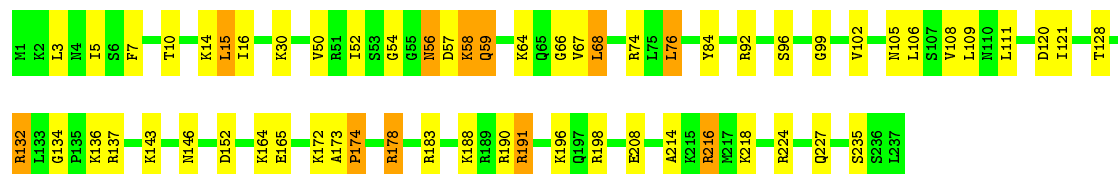
- Molecule 57: uS7

Chain FF: 



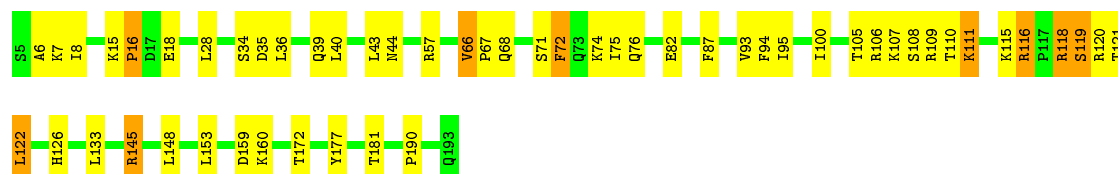
- Molecule 58: eS6

Chain GG: 

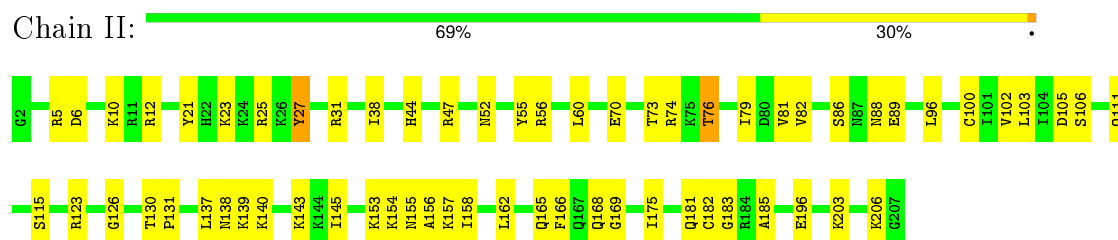


- Molecule 59: eS7

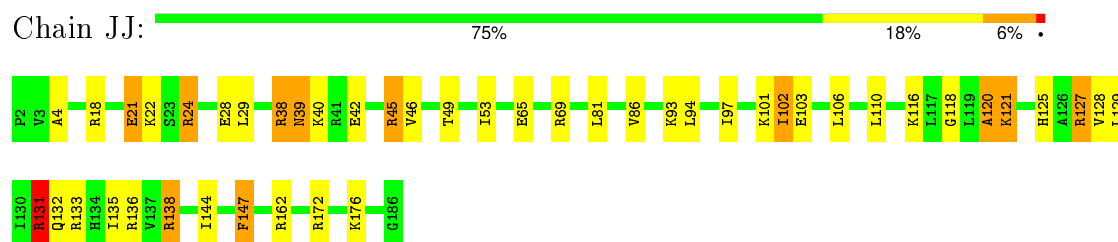
Chain HH: 



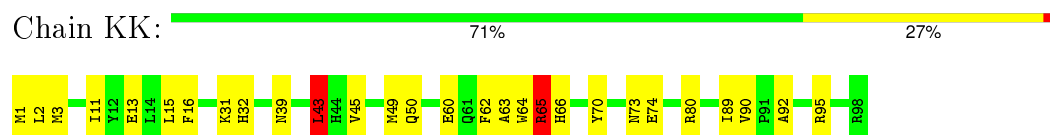
- Molecule 60: eS8



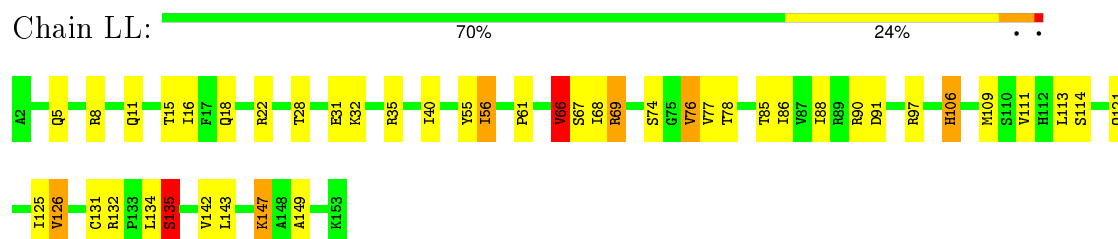
- Molecule 61: uS4



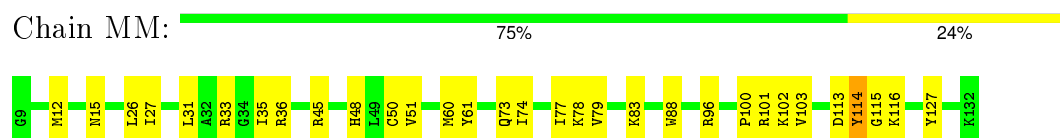
- Molecule 62: eS10



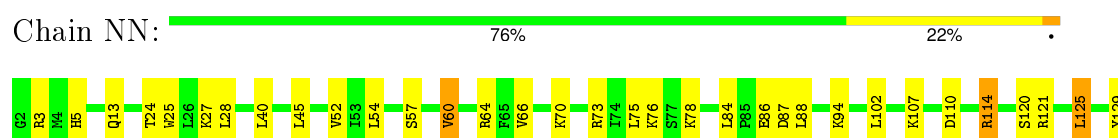
- Molecule 63: uS17



- Molecule 64: eS12



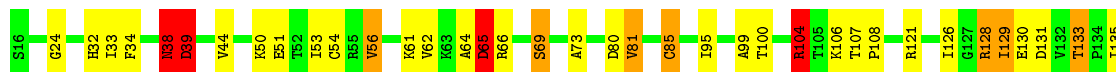
- Molecule 65: uS15





• Molecule 66: uS11

Chain OO: 67% 23% 7% •



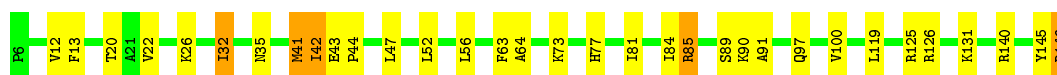
• Molecule 67: uS19

Chain PP: 75% 21% •



• Molecule 68: uS9

Chain QQ: 77% 20% •



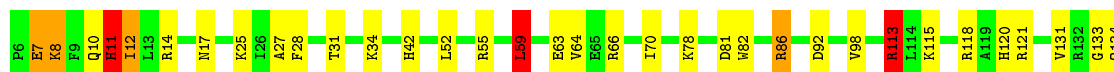
• Molecule 69: eS17

Chain RR: 78% 19% •



• Molecule 70: uS13

Chain SS: 74% 20% • •




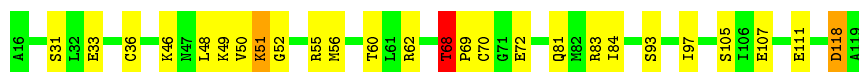
• Molecule 71: eS19

Chain TT: 79% 16% 5% •




• Molecule 72: uS10

Chain UU:  75% 22% ..



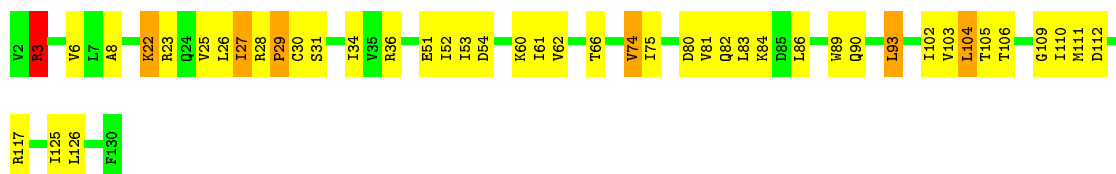
- Molecule 73: eS21

Chain VV:  73% 24% .



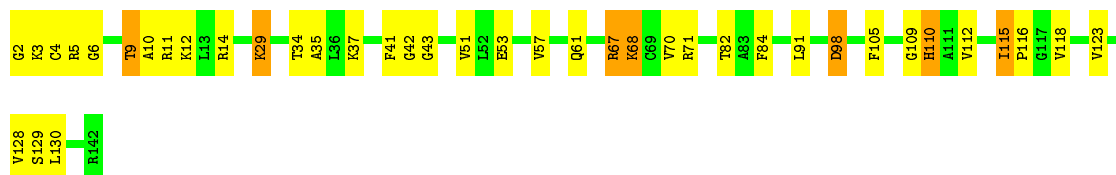
- Molecule 74: uS8

Chain WW:  65% 29% 5% .



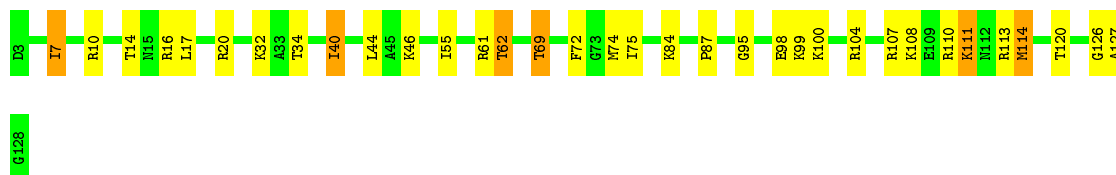
- Molecule 75: uS12

Chain XX:  72% 23% 5%




- Molecule 76: eS24

Chain YY:  73% 22% 5%




- Molecule 77: eS25

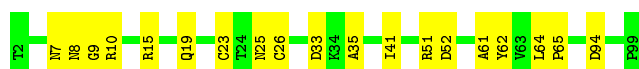
Chain ZZ:  77% 23%



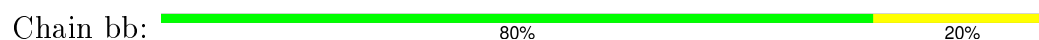
- Molecule 78: eS26

Chain aa:  81% 19%

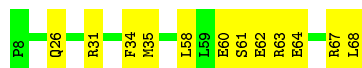
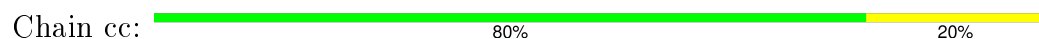




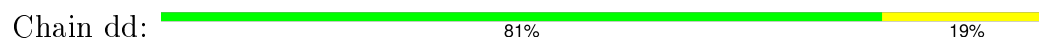
• Molecule 79: eS27



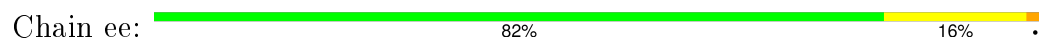
• Molecule 80: eS28



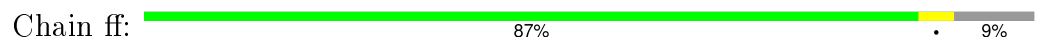
• Molecule 81: uS14



• Molecule 82: eS30



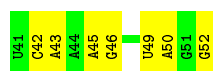
• Molecule 83: eS31



• Molecule 84: RACK1



• Molecule 85: mRNA

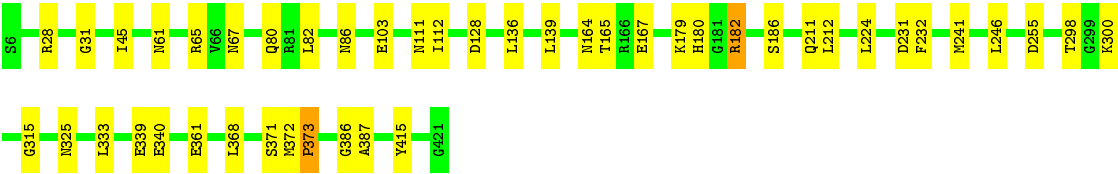


• Molecule 86: eRF1

Chain ii: 

89%

10%

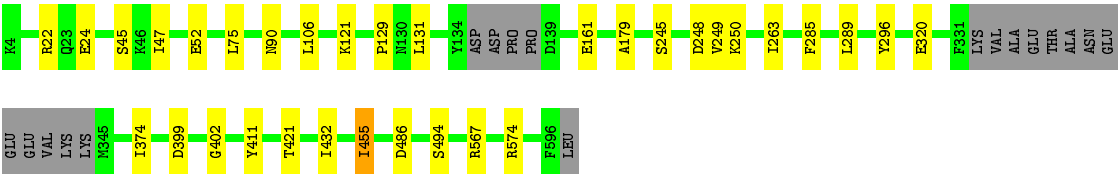


● Molecule 87: ABCE1

Chain jj: 

91%

5%



## 4 Experimental information

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, Not provided     | Depositor |
| Number of images                     | 20515                   | Depositor |
| Resolution determination method      | FSC 0.143               | Depositor |
| CTF correction method                | Not provided            | Depositor |
| Microscope                           | FEI TITAN KRIOS         | Depositor |
| Voltage (kV)                         | 300                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                      | Depositor |
| Minimum defocus (nm)                 | 1700                    | Depositor |
| Maximum defocus (nm)                 | 3600                    | Depositor |
| Magnification                        | 59000                   | Depositor |
| Image detector                       | FEI FALCON II (4k x 4k) | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SF4, ADP

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | # $ Z  > 2$ | RMSZ        | # $ Z  > 2$   |
| 1   | A     | 0.46         | 0/1906      | 0.79        | 0/2556        |
| 10  | J     | 0.38         | 0/1376      | 0.73        | 0/1841        |
| 11  | L     | 0.41         | 0/1734      | 0.79        | 0/2317        |
| 12  | M     | 0.37         | 0/1158      | 0.74        | 0/1547        |
| 13  | N     | 0.43         | 0/1746      | 0.83        | 0/2338        |
| 14  | O     | 0.40         | 0/1671      | 0.77        | 0/2234        |
| 15  | P     | 0.42         | 0/1268      | 0.75        | 0/1701        |
| 16  | Q     | 0.41         | 0/1530      | 0.81        | 1/2041 (0.0%) |
| 17  | R     | 0.41         | 0/1524      | 0.79        | 0/2013        |
| 18  | S     | 0.40         | 0/1493      | 0.85        | 3/2002 (0.1%) |
| 19  | T     | 0.41         | 0/1326      | 0.72        | 0/1770        |
| 2   | B     | 0.40         | 0/3216      | 0.78        | 1/4311 (0.0%) |
| 20  | U     | 0.41         | 0/822       | 0.68        | 0/1103        |
| 21  | V     | 0.40         | 0/993       | 0.73        | 0/1332        |
| 22  | W     | 0.48         | 0/541       | 0.83        | 1/720 (0.1%)  |
| 23  | X     | 0.42         | 0/993       | 0.74        | 0/1334        |
| 24  | Y     | 0.37         | 0/1132      | 0.80        | 2/1504 (0.1%) |
| 25  | Z     | 0.39         | 0/1130      | 0.72        | 0/1507        |
| 26  | a     | 0.40         | 0/1191      | 0.79        | 0/1590        |
| 27  | b     | 0.44         | 0/619       | 0.73        | 0/818         |
| 28  | c     | 0.36         | 0/742       | 0.69        | 0/996         |
| 29  | d     | 0.38         | 0/903       | 0.81        | 1/1216 (0.1%) |
| 3   | C     | 0.43         | 0/2938      | 0.80        | 5/3946 (0.1%) |
| 30  | e     | 0.47         | 0/1071      | 0.85        | 0/1429        |
| 31  | f     | 0.52         | 0/895       | 0.87        | 0/1198        |
| 32  | g     | 0.42         | 0/916       | 0.81        | 1/1220 (0.1%) |
| 33  | h     | 0.36         | 0/1021      | 0.77        | 1/1348 (0.1%) |
| 34  | i     | 0.40         | 0/841       | 0.82        | 2/1112 (0.2%) |
| 35  | j     | 0.45         | 0/720       | 0.93        | 1/952 (0.1%)  |
| 36  | k     | 0.37         | 0/575       | 0.68        | 0/761         |
| 37  | l     | 0.50         | 0/454       | 0.84        | 0/599         |
| 38  | m     | 0.37         | 0/435       | 0.76        | 0/575         |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >2        | RMSZ        | # Z  >2          |
| 39  | n     | 0.41         | 0/223          | 0.91        | 0/284            |
| 4   | D     | 0.37         | 0/2432         | 0.70        | 2/3257 (0.1%)    |
| 40  | o     | 0.39         | 0/864          | 0.75        | 0/1140           |
| 41  | p     | 0.42         | 0/718          | 0.71        | 0/953            |
| 42  | r     | 0.48         | 0/1017         | 0.80        | 1/1364 (0.1%)    |
| 43  | s     | 0.38         | 0/1547         | 0.58        | 0/2088           |
| 44  | t     | 0.41         | 0/1257         | 0.69        | 0/1697           |
| 45  | 1     | 0.45         | 0/129          | 0.72        | 0/173            |
| 46  | 2     | 0.26         | 0/1805         | 0.72        | 1/2809 (0.0%)    |
| 47  | 3     | 0.36         | 0/1777         | 0.97        | 10/2763 (0.4%)   |
| 48  | 5     | 0.37         | 4/87790 (0.0%) | 0.79        | 75/136937 (0.1%) |
| 49  | 7     | 0.30         | 0/2858         | 0.69        | 0/4455           |
| 5   | E     | 0.46         | 0/1936         | 0.82        | 2/2600 (0.1%)    |
| 50  | 8     | 0.36         | 0/3701         | 0.74        | 0/5766           |
| 51  | 9     | 0.32         | 1/41013 (0.0%) | 0.79        | 45/63919 (0.1%)  |
| 52  | AA    | 0.36         | 0/1679         | 0.70        | 0/2283           |
| 53  | BB    | 0.38         | 0/1756         | 0.77        | 4/2350 (0.2%)    |
| 54  | CC    | 0.41         | 0/1730         | 0.76        | 1/2344 (0.0%)    |
| 55  | DD    | 0.37         | 0/1792         | 0.72        | 0/2412           |
| 56  | EE    | 0.39         | 0/2115         | 0.78        | 0/2843           |
| 57  | FF    | 0.49         | 0/1531         | 0.78        | 1/2059 (0.0%)    |
| 58  | GG    | 0.37         | 0/1946         | 0.78        | 0/2590           |
| 59  | HH    | 0.44         | 0/1544         | 0.72        | 1/2068 (0.0%)    |
| 6   | F     | 0.40         | 0/1905         | 0.75        | 1/2539 (0.0%)    |
| 60  | II    | 0.41         | 0/1715         | 0.78        | 0/2287           |
| 61  | JJ    | 0.41         | 0/1550         | 0.88        | 4/2069 (0.2%)    |
| 62  | KK    | 0.47         | 0/851          | 0.73        | 0/1147           |
| 63  | LL    | 0.40         | 0/1259         | 0.78        | 0/1684           |
| 64  | MM    | 0.42         | 0/968          | 0.64        | 0/1296           |
| 65  | NN    | 0.39         | 0/1232         | 0.77        | 0/1656           |
| 66  | OO    | 0.42         | 0/1029         | 0.88        | 1/1380 (0.1%)    |
| 67  | PP    | 0.39         | 0/1079         | 0.76        | 0/1437           |
| 68  | QQ    | 0.37         | 0/1142         | 0.70        | 0/1528           |
| 69  | RR    | 0.42         | 0/1060         | 0.71        | 0/1421           |
| 7   | G     | 0.38         | 0/1967         | 0.73        | 1/2647 (0.0%)    |
| 70  | SS    | 0.38         | 0/1157         | 0.84        | 1/1548 (0.1%)    |
| 71  | TT    | 0.43         | 0/1120         | 0.78        | 2/1499 (0.1%)    |
| 72  | UU    | 0.36         | 0/831          | 0.71        | 0/1115           |
| 73  | VV    | 0.39         | 0/645          | 0.75        | 0/865            |
| 74  | WW    | 0.38         | 0/1051         | 0.79        | 0/1406           |
| 75  | XX    | 0.38         | 0/1116         | 0.80        | 0/1490           |
| 76  | YY    | 0.39         | 0/1040         | 0.74        | 0/1382           |
| 77  | ZZ    | 0.37         | 0/604          | 0.75        | 0/810            |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >2         | RMSZ        | # Z  >2           |
| 78  | aa    | 0.39         | 0/794           | 0.83        | 0/1065            |
| 79  | bb    | 0.37         | 0/665           | 0.67        | 0/891             |
| 8   | H     | 0.37         | 0/1535          | 0.71        | 0/2063            |
| 80  | cc    | 0.36         | 0/478           | 0.78        | 0/640             |
| 81  | dd    | 0.40         | 0/455           | 0.80        | 0/603             |
| 82  | ee    | 0.46         | 0/462           | 0.75        | 0/607             |
| 83  | ff    | 0.39         | 0/531           | 0.62        | 0/703             |
| 84  | gg    | 0.37         | 0/2493          | 0.65        | 0/3394            |
| 85  | hh    | 0.29         | 0/287           | 0.76        | 0/445             |
| 86  | ii    | 0.39         | 0/3333          | 0.63        | 2/4483 (0.0%)     |
| 87  | jj    | 0.47         | 1/4625 (0.0%)   | 0.58        | 0/6238            |
| 9   | I     | 0.41         | 0/1693          | 0.69        | 0/2260            |
| All | All   | 0.38         | 6/242712 (0.0%) | 0.78        | 174/355683 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 11  | L     | 0                   | 3                   |
| 17  | R     | 0                   | 1                   |
| 18  | S     | 0                   | 2                   |
| 19  | T     | 0                   | 1                   |
| 2   | B     | 0                   | 4                   |
| 20  | U     | 0                   | 1                   |
| 24  | Y     | 0                   | 1                   |
| 3   | C     | 0                   | 2                   |
| 31  | f     | 0                   | 1                   |
| 4   | D     | 0                   | 1                   |
| 42  | r     | 0                   | 2                   |
| 48  | 5     | 0                   | 1                   |
| 5   | E     | 0                   | 1                   |
| 51  | 9     | 0                   | 1                   |
| 52  | AA    | 0                   | 1                   |
| 56  | EE    | 0                   | 2                   |
| 57  | FF    | 0                   | 2                   |
| 59  | HH    | 0                   | 1                   |
| 60  | II    | 0                   | 1                   |
| 61  | JJ    | 0                   | 2                   |
| 66  | OO    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 68  | QQ    | 0                   | 1                   |
| 7   | G     | 0                   | 1                   |
| 70  | SS    | 0                   | 1                   |
| 71  | TT    | 0                   | 1                   |
| 72  | UU    | 0                   | 2                   |
| 73  | VV    | 0                   | 1                   |
| 74  | WW    | 0                   | 2                   |
| 75  | XX    | 0                   | 1                   |
| 78  | aa    | 0                   | 1                   |
| 86  | ii    | 0                   | 3                   |
| 9   | I     | 0                   | 2                   |
| All | All   | 0                   | 49                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 48  | 5     | 1965 | G    | O3'-P | -23.01 | 1.33        | 1.61     |
| 87  | jj    | 121  | LYS  | CE-NZ | 19.94  | 1.99        | 1.49     |
| 51  | 9     | 908  | A    | O3'-P | 8.98   | 1.72        | 1.61     |
| 48  | 5     | 1847 | C    | O3'-P | -6.16  | 1.53        | 1.61     |
| 48  | 5     | 957  | G    | O3'-P | 5.62   | 1.67        | 1.61     |
| 48  | 5     | 1358 | G    | O3'-P | 5.10   | 1.67        | 1.61     |

All (174) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 51  | 9     | 909  | G    | O5'-P-OP2   | -16.21 | 91.11       | 105.70   |
| 47  | 3     | 70   | G    | N9-C1'-C2'  | -13.18 | 96.87       | 114.00   |
| 48  | 5     | 3753 | G    | N9-C1'-C2'  | -11.91 | 98.52       | 114.00   |
| 51  | 9     | 1235 | G    | N9-C1'-C2'  | -11.46 | 99.11       | 114.00   |
| 48  | 5     | 3718 | A    | N9-C1'-C2'  | -10.30 | 100.61      | 114.00   |
| 48  | 5     | 1358 | G    | C4'-C3'-O3' | 10.21  | 133.41      | 113.00   |
| 51  | 9     | 1386 | A    | N9-C1'-C2'  | -10.19 | 100.76      | 114.00   |
| 51  | 9     | 1212 | G    | N9-C1'-C2'  | -10.02 | 100.98      | 114.00   |
| 48  | 5     | 1357 | C    | C4'-C3'-O3' | 9.68   | 132.37      | 113.00   |
| 24  | Y     | 87   | ARG  | NE-CZ-NH2   | 9.17   | 124.89      | 120.30   |
| 48  | 5     | 4975 | G    | C2'-C3'-O3' | 8.96   | 129.21      | 109.50   |
| 51  | 9     | 1294 | G    | N9-C1'-C2'  | -8.95  | 102.15      | 112.00   |
| 47  | 3     | 38   | A    | N9-C1'-C2'  | -8.89  | 102.22      | 112.00   |
| 47  | 3     | 30   | G    | N9-C1'-C2'  | -8.83  | 102.28      | 112.00   |
| 53  | BB    | 136  | ARG  | NE-CZ-NH2   | 8.82   | 124.71      | 120.30   |
| 22  | W     | 44   | ARG  | NE-CZ-NH1   | 8.56   | 124.58      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 90   | G    | C2'-C3'-O3' | 8.38  | 127.95      | 109.50   |
| 48  | 5     | 4528 | G    | C2'-C3'-O3' | 8.37  | 127.90      | 109.50   |
| 48  | 5     | 3888 | G    | C2'-C3'-O3' | 8.31  | 127.79      | 109.50   |
| 47  | 3     | 70   | G    | C4'-C3'-O3' | 8.30  | 129.60      | 113.00   |
| 51  | 9     | 1394 | G    | C2'-C3'-O3' | 8.28  | 127.71      | 109.50   |
| 48  | 5     | 1969 | G    | N9-C1'-C2'  | -8.26 | 102.91      | 112.00   |
| 70  | SS    | 113  | ARG  | NE-CZ-NH1   | 8.20  | 124.40      | 120.30   |
| 61  | JJ    | 127  | ARG  | NE-CZ-NH1   | 8.12  | 124.36      | 120.30   |
| 48  | 5     | 4948 | C    | C2'-C3'-O3' | 8.04  | 127.19      | 109.50   |
| 51  | 9     | 1385 | G    | N9-C1'-C2'  | -8.01 | 103.19      | 112.00   |
| 18  | S     | 83   | ARG  | NE-CZ-NH2   | 7.99  | 124.29      | 120.30   |
| 48  | 5     | 1211 | G    | C2'-C3'-O3' | 7.95  | 126.98      | 109.50   |
| 48  | 5     | 3697 | U    | C2'-C3'-O3' | 7.90  | 126.87      | 109.50   |
| 35  | j     | 63   | ARG  | NE-CZ-NH1   | 7.84  | 124.22      | 120.30   |
| 48  | 5     | 1455 | G    | C2'-C3'-O3' | 7.78  | 126.60      | 109.50   |
| 51  | 9     | 1235 | G    | C4'-C3'-O3' | 7.73  | 128.47      | 113.00   |
| 61  | JJ    | 131  | ARG  | NE-CZ-NH1   | 7.71  | 124.15      | 120.30   |
| 48  | 5     | 2858 | A    | N9-C1'-C2'  | -7.65 | 103.59      | 112.00   |
| 48  | 5     | 2858 | A    | C4'-C3'-O3' | 7.62  | 128.23      | 113.00   |
| 47  | 3     | 39   | U    | N1-C1'-C2'  | -7.58 | 103.66      | 112.00   |
| 51  | 9     | 1681 | U    | N1-C1'-C2'  | -7.56 | 103.68      | 112.00   |
| 48  | 5     | 1292 | C    | C2'-C3'-O3' | 7.52  | 126.05      | 109.50   |
| 3   | C     | 342  | ARG  | NE-CZ-NH1   | 7.51  | 124.05      | 120.30   |
| 48  | 5     | 3718 | A    | C4'-C3'-O3' | 7.50  | 128.00      | 113.00   |
| 51  | 9     | 322  | C    | N1-C1'-C2'  | -7.45 | 103.80      | 112.00   |
| 51  | 9     | 1448 | A    | N9-C1'-C2'  | -7.42 | 103.84      | 112.00   |
| 51  | 9     | 1641 | A    | O5'-P-OP1   | -7.38 | 99.06       | 105.70   |
| 48  | 5     | 275  | C    | C2'-C3'-O3' | 7.36  | 125.68      | 109.50   |
| 48  | 5     | 5060 | A    | C2'-C3'-O3' | 7.33  | 125.62      | 109.50   |
| 48  | 5     | 125  | C    | C2'-C3'-O3' | 7.32  | 125.61      | 109.50   |
| 48  | 5     | 1477 | C    | C2'-C3'-O3' | 7.27  | 125.50      | 109.50   |
| 48  | 5     | 2797 | C    | N1-C1'-C2'  | -7.26 | 104.02      | 112.00   |
| 71  | TT    | 56   | ARG  | NE-CZ-NH1   | 7.26  | 123.93      | 120.30   |
| 61  | JJ    | 24   | ARG  | NE-CZ-NH1   | 7.24  | 123.92      | 120.30   |
| 48  | 5     | 5061 | A    | C2'-C3'-O3' | 7.19  | 125.33      | 109.50   |
| 51  | 9     | 1144 | A    | N9-C1'-C2'  | 7.18  | 123.34      | 114.00   |
| 48  | 5     | 47   | A    | C4'-C3'-O3' | 7.18  | 127.36      | 113.00   |
| 48  | 5     | 2695 | A    | C2'-C3'-O3' | 7.14  | 125.21      | 109.50   |
| 51  | 9     | 1268 | C    | N1-C1'-C2'  | -7.13 | 104.15      | 112.00   |
| 48  | 5     | 406  | C    | C2'-C3'-O3' | 7.13  | 125.19      | 109.50   |
| 48  | 5     | 2027 | U    | N1-C1'-C2'  | -7.13 | 104.16      | 112.00   |
| 48  | 5     | 5059 | C    | C2'-C3'-O3' | 7.13  | 125.18      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 86  | ii    | 182  | ARG  | NE-CZ-NH1   | 7.12  | 123.86      | 120.30   |
| 47  | 3     | 1    | G    | C5'-C4'-O4' | 7.08  | 117.59      | 109.10   |
| 51  | 9     | 1455 | A    | N9-C1'-C2'  | -7.07 | 104.22      | 112.00   |
| 51  | 9     | 102  | A    | C2'-C3'-O3' | 7.04  | 124.99      | 109.50   |
| 48  | 5     | 1485 | C    | C2'-C3'-O3' | 6.93  | 124.80      | 113.70   |
| 61  | JJ    | 131  | ARG  | NE-CZ-NH2   | -6.91 | 116.85      | 120.30   |
| 51  | 9     | 642  | U    | C4'-C3'-O3' | 6.88  | 126.76      | 113.00   |
| 51  | 9     | 666  | U    | N1-C1'-C2'  | 6.84  | 122.89      | 114.00   |
| 48  | 5     | 1279 | A    | C2'-C3'-O3' | 6.80  | 124.58      | 113.70   |
| 48  | 5     | 2046 | G    | C2'-C3'-O3' | 6.76  | 124.52      | 113.70   |
| 48  | 5     | 1236 | C    | C2'-C3'-O3' | 6.71  | 124.43      | 113.70   |
| 48  | 5     | 977  | C    | C2'-C3'-O3' | 6.68  | 124.39      | 113.70   |
| 48  | 5     | 4885 | U    | C2'-C3'-O3' | 6.66  | 124.35      | 113.70   |
| 48  | 5     | 93   | G    | C4'-C3'-O3' | 6.64  | 126.29      | 113.00   |
| 34  | i     | 25   | ARG  | NE-CZ-NH1   | 6.54  | 123.57      | 120.30   |
| 51  | 9     | 312  | G    | C2'-C3'-O3' | 6.53  | 124.15      | 113.70   |
| 48  | 5     | 1818 | G    | C2'-C3'-O3' | 6.51  | 124.12      | 113.70   |
| 51  | 9     | 1447 | G    | N9-C1'-C2'  | -6.49 | 104.86      | 112.00   |
| 48  | 5     | 2083 | C    | C4'-C3'-O3' | 6.44  | 125.87      | 113.00   |
| 51  | 9     | 1386 | A    | C4'-C3'-O3' | 6.44  | 125.88      | 113.00   |
| 51  | 9     | 1060 | A    | N9-C1'-C2'  | 6.42  | 122.34      | 114.00   |
| 48  | 5     | 93   | G    | N9-C1'-C2'  | -6.39 | 104.97      | 112.00   |
| 47  | 3     | 69   | G    | O4'-C1'-N9  | 6.39  | 113.31      | 108.20   |
| 48  | 5     | 3657 | U    | C2'-C3'-O3' | 6.36  | 123.87      | 113.70   |
| 4   | D     | 22   | ARG  | NE-CZ-NH1   | 6.34  | 123.47      | 120.30   |
| 48  | 5     | 1474 | C    | C2'-C3'-O3' | 6.32  | 123.82      | 113.70   |
| 5   | E     | 208  | LEU  | CA-CB-CG    | 6.32  | 129.84      | 115.30   |
| 48  | 5     | 1500 | A    | C2'-C3'-O3' | 6.29  | 123.76      | 113.70   |
| 51  | 9     | 1    | U    | C5'-C4'-O4' | 6.29  | 116.64      | 109.10   |
| 48  | 5     | 1398 | A    | C2'-C3'-O3' | 6.28  | 123.74      | 113.70   |
| 51  | 9     | 110  | U    | C2'-C3'-O3' | 6.28  | 123.74      | 113.70   |
| 48  | 5     | 2123 | C    | C2'-C3'-O3' | 6.23  | 123.67      | 113.70   |
| 48  | 5     | 1380 | G    | N9-C1'-C2'  | 6.22  | 122.09      | 114.00   |
| 48  | 5     | 1969 | G    | C4'-C3'-O3' | 6.22  | 125.45      | 113.00   |
| 48  | 5     | 1239 | C    | C2'-C3'-O3' | 6.21  | 123.64      | 113.70   |
| 48  | 5     | 2632 | U    | N1-C1'-C2'  | 6.17  | 122.02      | 114.00   |
| 51  | 9     | 322  | C    | C2'-C3'-O3' | -6.15 | 95.97       | 109.50   |
| 51  | 9     | 1211 | G    | N9-C1'-C2'  | -6.12 | 105.27      | 112.00   |
| 51  | 9     | 62   | G    | C2'-C3'-O3' | 6.09  | 123.45      | 113.70   |
| 51  | 9     | 434  | G    | C2'-C3'-O3' | 6.05  | 123.38      | 113.70   |
| 48  | 5     | 1072 | C    | N1-C1'-C2'  | 6.03  | 121.84      | 114.00   |
| 48  | 5     | 1672 | U    | N1-C1'-C2'  | 6.02  | 121.83      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | 5     | 1848 | C    | C2'-C3'-O3' | 6.01  | 123.31      | 113.70   |
| 29  | d     | 78   | ARG  | NE-CZ-NH1   | 5.98  | 123.29      | 120.30   |
| 48  | 5     | 1390 | G    | C2'-C3'-O3' | 5.93  | 123.19      | 113.70   |
| 34  | i     | 85   | ARG  | NE-CZ-NH1   | 5.93  | 123.26      | 120.30   |
| 48  | 5     | 1965 | G    | P-O3'-C3'   | 5.90  | 126.78      | 119.70   |
| 48  | 5     | 1696 | C    | C2'-C3'-O3' | 5.90  | 123.13      | 113.70   |
| 51  | 9     | 1419 | C    | C2'-C3'-O3' | 5.89  | 123.12      | 113.70   |
| 16  | Q     | 104  | ARG  | NE-CZ-NH1   | 5.87  | 123.23      | 120.30   |
| 48  | 5     | 978  | G    | C2'-C3'-O3' | 5.81  | 123.00      | 113.70   |
| 48  | 5     | 4872 | G    | C2'-C3'-O3' | 5.78  | 122.95      | 113.70   |
| 5   | E     | 72   | PRO  | N-CA-CB     | 5.78  | 110.24      | 103.30   |
| 48  | 5     | 4951 | G    | C2'-C3'-O3' | 5.77  | 122.93      | 113.70   |
| 48  | 5     | 1329 | G    | C2'-C3'-O3' | 5.76  | 122.91      | 113.70   |
| 48  | 5     | 4975 | G    | C4'-C3'-O3' | -5.72 | 97.39       | 109.40   |
| 48  | 5     | 215  | C    | C2'-C3'-O3' | 5.69  | 122.80      | 113.70   |
| 51  | 9     | 1824 | A    | C2'-C3'-O3' | 5.67  | 122.77      | 113.70   |
| 3   | C     | 98   | GLY  | N-CA-C      | -5.65 | 98.97       | 113.10   |
| 47  | 3     | 1    | G    | C5'-C4'-C3' | 5.63  | 125.00      | 116.00   |
| 51  | 9     | 1    | U    | C5'-C4'-C3' | 5.62  | 124.99      | 116.00   |
| 51  | 9     | 1234 | C    | N1-C1'-C2'  | -5.60 | 105.83      | 112.00   |
| 6   | F     | 91   | LEU  | CA-CB-CG    | 5.54  | 128.05      | 115.30   |
| 18  | S     | 83   | ARG  | NE-CZ-NH1   | -5.51 | 117.55      | 120.30   |
| 2   | B     | 36   | ASP  | C-N-CD      | 5.50  | 139.96      | 128.40   |
| 51  | 9     | 1137 | U    | C2'-C3'-O3' | 5.49  | 122.48      | 113.70   |
| 57  | FF    | 135  | ARG  | NE-CZ-NH2   | -5.48 | 117.56      | 120.30   |
| 47  | 3     | 29   | A    | N9-C1'-C2'  | -5.46 | 105.99      | 112.00   |
| 48  | 5     | 979  | C    | C2'-C3'-O3' | 5.46  | 122.44      | 113.70   |
| 48  | 5     | 4473 | A    | N9-C1'-C2'  | 5.46  | 121.09      | 114.00   |
| 48  | 5     | 2054 | U    | N1-C1'-C2'  | 5.45  | 121.08      | 114.00   |
| 53  | BB    | 136  | ARG  | CG-CD-NE    | 5.45  | 123.23      | 111.80   |
| 71  | TT    | 56   | ARG  | NE-CZ-NH2   | -5.42 | 117.59      | 120.30   |
| 47  | 3     | 30   | G    | C4'-C3'-O3' | 5.41  | 123.82      | 113.00   |
| 48  | 5     | 2028 | C    | N1-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 48  | 5     | 957  | G    | P-O3'-C3'   | 5.40  | 126.19      | 119.70   |
| 51  | 9     | 1385 | G    | C4'-C3'-O3' | 5.38  | 123.77      | 113.00   |
| 59  | HH    | 118  | ARG  | NE-CZ-NH1   | 5.38  | 122.99      | 120.30   |
| 24  | Y     | 75   | ARG  | NE-CZ-NH1   | 5.38  | 122.99      | 120.30   |
| 48  | 5     | 1365 | C    | C4'-C3'-O3' | 5.37  | 123.75      | 113.00   |
| 51  | 9     | 1144 | A    | C8-N9-C1'   | -5.35 | 118.07      | 127.70   |
| 51  | 9     | 844  | U    | C5'-C4'-O4' | 5.34  | 115.51      | 109.10   |
| 86  | ii    | 372  | MET  | C-N-CD      | 5.33  | 139.60      | 128.40   |
| 66  | OO    | 146  | ARG  | NE-CZ-NH2   | -5.31 | 117.64      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 51  | 9     | 1212 | G    | C4'-C3'-O3' | 5.29  | 123.59      | 113.00   |
| 53  | BB    | 136  | ARG  | NE-CZ-NH1   | -5.29 | 117.65      | 120.30   |
| 48  | 5     | 486  | C    | C2'-C3'-O3' | 5.29  | 122.16      | 113.70   |
| 51  | 9     | 909  | G    | O5'-P-OP1   | 5.29  | 117.05      | 110.70   |
| 48  | 5     | 1266 | G    | C2'-C3'-O3' | 5.28  | 122.15      | 113.70   |
| 48  | 5     | 3715 | U    | N1-C1'-C2'  | -5.27 | 106.20      | 112.00   |
| 48  | 5     | 2586 | G    | N9-C1'-C2'  | 5.25  | 120.82      | 114.00   |
| 3   | C     | 262  | ASP  | CB-CG-OD2   | 5.23  | 123.00      | 118.30   |
| 18  | S     | 83   | ARG  | CG-CD-NE    | 5.22  | 122.76      | 111.80   |
| 33  | h     | 22   | ASP  | CB-CG-OD2   | 5.21  | 122.98      | 118.30   |
| 51  | 9     | 1647 | A    | C2'-C3'-O3' | 5.18  | 122.00      | 113.70   |
| 51  | 9     | 1144 | A    | C4-N9-C1'   | 5.16  | 135.58      | 126.30   |
| 7   | G     | 231  | ASP  | CB-CG-OD2   | 5.15  | 122.94      | 118.30   |
| 51  | 9     | 1408 | U    | O5'-P-OP1   | -5.13 | 101.09      | 105.70   |
| 48  | 5     | 4731 | G    | N9-C1'-C2'  | 5.11  | 120.65      | 114.00   |
| 42  | r     | 17   | LEU  | CA-CB-CG    | 5.11  | 127.05      | 115.30   |
| 48  | 5     | 2661 | U    | C2'-C3'-O3' | 5.11  | 121.88      | 113.70   |
| 53  | BB    | 136  | ARG  | CD-NE-CZ    | 5.10  | 130.74      | 123.60   |
| 48  | 5     | 4481 | U    | C5'-C4'-O4' | 5.09  | 115.21      | 109.10   |
| 48  | 5     | 4965 | U    | C2'-C3'-O3' | 5.07  | 121.81      | 113.70   |
| 51  | 9     | 532  | C    | C2'-C3'-O3' | 5.06  | 121.79      | 113.70   |
| 51  | 9     | 1109 | C    | N1-C1'-C2'  | 5.05  | 120.57      | 114.00   |
| 3   | C     | 67   | TRP  | N-CA-C      | -5.04 | 97.39       | 111.00   |
| 48  | 5     | 1755 | C    | C2'-C3'-O3' | 5.04  | 121.77      | 113.70   |
| 51  | 9     | 488  | U    | N1-C1'-C2'  | 5.04  | 120.55      | 114.00   |
| 3   | C     | 45   | ARG  | NE-CZ-NH1   | 5.04  | 122.82      | 120.30   |
| 32  | g     | 66   | ARG  | NE-CZ-NH1   | 5.04  | 122.82      | 120.30   |
| 46  | 2     | 34   | A    | N9-C1'-C2'  | -5.03 | 106.46      | 112.00   |
| 54  | CC    | 233  | LEU  | CA-CB-CG    | 5.03  | 126.87      | 115.30   |
| 51  | 9     | 1354 | G    | C2'-C3'-O3' | 5.03  | 121.75      | 113.70   |
| 4   | D     | 22   | ARG  | CG-CD-NE    | 5.02  | 122.33      | 111.80   |
| 48  | 5     | 2246 | C    | C2'-C3'-O3' | 5.01  | 121.72      | 113.70   |

There are no chirality outliers.

All (49) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 48  | 5     | 2793 | G    | Sidechain |
| 51  | 9     | 1448 | A    | Sidechain |
| 1   | A     | 196  | TRP  | Peptide   |
| 52  | AA    | 73   | ASP  | Peptide   |
| 2   | B     | 17   | LEU  | Peptide   |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 2          | B            | 257        | TRP         | Peptide      |
| 2          | B            | 258        | HIS         | Peptide      |
| 2          | B            | 351        | LEU         | Peptide      |
| 3          | C            | 245        | HIS         | Peptide      |
| 3          | C            | 339        | THR         | Peptide      |
| 4          | D            | 36         | LEU         | Peptide      |
| 5          | E            | 123        | SER         | Peptide      |
| 56         | EE           | 129        | ILE         | Peptide      |
| 56         | EE           | 155        | LYS         | Peptide      |
| 57         | FF           | 42         | LYS         | Peptide      |
| 57         | FF           | 43         | GLU         | Peptide      |
| 7          | G            | 238        | GLY         | Peptide      |
| 59         | HH           | 111        | LYS         | Peptide      |
| 9          | I            | 188        | LYS         | Peptide      |
| 9          | I            | 202        | ASN         | Peptide      |
| 60         | II           | 154        | LYS         | Peptide      |
| 61         | JJ           | 38         | ARG         | Peptide      |
| 61         | JJ           | 93         | LYS         | Peptide      |
| 11         | L            | 27         | ASN         | Peptide      |
| 11         | L            | 46         | ILE         | Peptide      |
| 11         | L            | 66         | TYR         | Peptide      |
| 66         | OO           | 104        | ARG         | Peptide      |
| 68         | QQ           | 42         | ILE         | Peptide      |
| 17         | R            | 19         | LYS         | Peptide      |
| 18         | S            | 163        | HIS         | Peptide      |
| 18         | S            | 164        | LYS         | Peptide      |
| 70         | SS           | 11         | HIS         | Peptide      |
| 19         | T            | 26         | PRO         | Peptide      |
| 71         | TT           | 42         | HIS         | Peptide      |
| 20         | U            | 27         | HIS         | Peptide      |
| 72         | UU           | 68         | THR         | Peptide      |
| 72         | UU           | 72         | GLU         | Peptide      |
| 73         | VV           | 32         | ILE         | Peptide      |
| 74         | WW           | 27         | ILE         | Peptide      |
| 74         | WW           | 54         | ASP         | Peptide      |
| 75         | XX           | 98         | ASP         | Peptide      |
| 24         | Y            | 7          | VAL         | Peptide      |
| 78         | aa           | 7          | ASN         | Peptide      |
| 31         | f            | 105        | LEU         | Peptide      |
| 86         | ii           | 325        | ASN         | Peptide      |
| 86         | ii           | 371        | SER         | Peptide      |
| 86         | ii           | 373        | PRO         | Peptide      |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 42  | r     | 106 | LEU  | Peptide |
| 42  | r     | 70  | GLN  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1868  | 0        | 1959     | 31      | 0            |
| 2   | B     | 3148  | 0        | 3267     | 55      | 0            |
| 3   | C     | 2884  | 0        | 3062     | 45      | 0            |
| 4   | D     | 2386  | 0        | 2419     | 31      | 0            |
| 5   | E     | 1898  | 0        | 2035     | 66      | 0            |
| 6   | F     | 1870  | 0        | 1994     | 27      | 0            |
| 7   | G     | 1934  | 0        | 2087     | 32      | 0            |
| 8   | H     | 1516  | 0        | 1597     | 10      | 0            |
| 9   | I     | 1655  | 0        | 1704     | 45      | 0            |
| 10  | J     | 1353  | 0        | 1386     | 16      | 0            |
| 11  | L     | 1703  | 0        | 1820     | 22      | 0            |
| 12  | M     | 1137  | 0        | 1211     | 16      | 0            |
| 13  | N     | 1701  | 0        | 1749     | 18      | 0            |
| 14  | O     | 1638  | 0        | 1777     | 31      | 0            |
| 15  | P     | 1242  | 0        | 1269     | 12      | 0            |
| 16  | Q     | 1506  | 0        | 1623     | 14      | 0            |
| 17  | R     | 1508  | 0        | 1664     | 31      | 0            |
| 18  | S     | 1454  | 0        | 1496     | 14      | 0            |
| 19  | T     | 1298  | 0        | 1366     | 11      | 0            |
| 20  | U     | 808   | 0        | 831      | 5       | 0            |
| 21  | V     | 979   | 0        | 1039     | 5       | 0            |
| 22  | W     | 528   | 0        | 541      | 5       | 0            |
| 23  | X     | 976   | 0        | 1053     | 8       | 0            |
| 24  | Y     | 1115  | 0        | 1205     | 6       | 0            |
| 25  | Z     | 1107  | 0        | 1182     | 16      | 0            |
| 26  | a     | 1162  | 0        | 1209     | 0       | 0            |
| 27  | b     | 609   | 0        | 650      | 0       | 0            |
| 28  | c     | 732   | 0        | 769      | 0       | 0            |
| 29  | d     | 888   | 0        | 930      | 0       | 0            |
| 30  | e     | 1053  | 0        | 1147     | 0       | 0            |
| 31  | f     | 876   | 0        | 912      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | g     | 906   | 0        | 999      | 0       | 0            |
| 33  | h     | 1013  | 0        | 1147     | 0       | 0            |
| 34  | i     | 830   | 0        | 916      | 0       | 0            |
| 35  | j     | 705   | 0        | 738      | 0       | 0            |
| 36  | k     | 569   | 0        | 637      | 0       | 0            |
| 37  | l     | 444   | 0        | 483      | 0       | 0            |
| 38  | m     | 429   | 0        | 466      | 0       | 0            |
| 39  | n     | 222   | 0        | 264      | 0       | 0            |
| 40  | o     | 851   | 0        | 921      | 0       | 0            |
| 41  | p     | 708   | 0        | 756      | 0       | 0            |
| 42  | r     | 1001  | 0        | 1060     | 0       | 0            |
| 43  | s     | 1523  | 0        | 1577     | 0       | 0            |
| 44  | t     | 1238  | 0        | 1295     | 0       | 0            |
| 45  | 1     | 125   | 0        | 117      | 3       | 0            |
| 46  | 2     | 1616  | 0        | 824      | 18      | 0            |
| 47  | 3     | 1593  | 0        | 811      | 79      | 0            |
| 48  | 5     | 78486 | 0        | 39663    | 1322    | 0            |
| 49  | 7     | 2558  | 0        | 1296     | 27      | 0            |
| 50  | 8     | 3314  | 0        | 1683     | 53      | 0            |
| 51  | 9     | 36680 | 0        | 18529    | 615     | 0            |
| 52  | AA    | 1642  | 0        | 1646     | 22      | 0            |
| 53  | BB    | 1729  | 0        | 1803     | 15      | 0            |
| 54  | CC    | 1692  | 0        | 1780     | 22      | 0            |
| 55  | DD    | 1764  | 0        | 1863     | 8       | 0            |
| 56  | EE    | 2073  | 0        | 2175     | 45      | 0            |
| 57  | FF    | 1509  | 0        | 1562     | 28      | 0            |
| 58  | GG    | 1923  | 0        | 2089     | 29      | 0            |
| 59  | HH    | 1521  | 0        | 1616     | 20      | 0            |
| 60  | II    | 1686  | 0        | 1772     | 30      | 0            |
| 61  | JJ    | 1525  | 0        | 1640     | 22      | 0            |
| 62  | KK    | 827   | 0        | 854      | 7       | 0            |
| 63  | LL    | 1238  | 0        | 1315     | 17      | 0            |
| 64  | MM    | 958   | 0        | 993      | 3       | 0            |
| 65  | NN    | 1208  | 0        | 1294     | 8       | 0            |
| 66  | OO    | 1016  | 0        | 1039     | 14      | 0            |
| 67  | PP    | 1060  | 0        | 1120     | 13      | 0            |
| 68  | QQ    | 1124  | 0        | 1193     | 11      | 0            |
| 69  | RR    | 1047  | 0        | 1103     | 9       | 0            |
| 70  | SS    | 1139  | 0        | 1191     | 17      | 0            |
| 71  | TT    | 1102  | 0        | 1142     | 11      | 0            |
| 72  | UU    | 821   | 0        | 883      | 6       | 0            |
| 73  | VV    | 636   | 0        | 634      | 9       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 74  | WW    | 1034   | 0        | 1080     | 23      | 0            |
| 75  | XX    | 1098   | 0        | 1167     | 11      | 0            |
| 76  | YY    | 1023   | 0        | 1090     | 11      | 0            |
| 77  | ZZ    | 598    | 0        | 656      | 6       | 0            |
| 78  | aa    | 781    | 0        | 828      | 0       | 0            |
| 79  | bb    | 651    | 0        | 672      | 0       | 0            |
| 80  | cc    | 475    | 0        | 497      | 0       | 0            |
| 81  | dd    | 445    | 0        | 439      | 0       | 0            |
| 82  | ee    | 457    | 0        | 502      | 0       | 0            |
| 83  | ff    | 520    | 0        | 536      | 0       | 0            |
| 84  | gg    | 2436   | 0        | 2393     | 0       | 0            |
| 85  | hh    | 257    | 0        | 129      | 0       | 0            |
| 86  | ii    | 3280   | 0        | 3326     | 0       | 0            |
| 87  | jj    | 4543   | 0        | 4674     | 0       | 0            |
| 88  | 5     | 146    | 0        | 0        | 0       | 0            |
| 88  | 7     | 5      | 0        | 0        | 0       | 0            |
| 88  | 8     | 2      | 0        | 0        | 0       | 0            |
| 88  | 9     | 34     | 0        | 0        | 0       | 0            |
| 88  | B     | 1      | 0        | 0        | 0       | 0            |
| 88  | C     | 1      | 0        | 0        | 0       | 0            |
| 88  | I     | 1      | 0        | 0        | 0       | 0            |
| 88  | LL    | 1      | 0        | 0        | 0       | 0            |
| 88  | P     | 1      | 0        | 0        | 0       | 0            |
| 88  | V     | 1      | 0        | 0        | 0       | 0            |
| 88  | g     | 1      | 0        | 0        | 0       | 0            |
| 88  | hh    | 1      | 0        | 0        | 0       | 0            |
| 89  | aa    | 1      | 0        | 0        | 0       | 0            |
| 89  | dd    | 1      | 0        | 0        | 0       | 0            |
| 89  | ff    | 1      | 0        | 0        | 0       | 0            |
| 89  | g     | 1      | 0        | 0        | 0       | 0            |
| 89  | j     | 1      | 0        | 0        | 0       | 0            |
| 89  | m     | 1      | 0        | 0        | 0       | 0            |
| 89  | o     | 1      | 0        | 0        | 0       | 0            |
| 89  | p     | 1      | 0        | 0        | 0       | 0            |
| 90  | jj    | 16     | 0        | 0        | 0       | 0            |
| 91  | jj    | 54     | 0        | 24       | 0       | 0            |
| All | All   | 226454 | 0        | 169855   | 2802    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2802) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:9:1137:U:O4    | 51:9:1148:A:N1    | 1.61                     | 1.34              |
| 48:5:976:G:H2'    | 48:5:977:C:O4'    | 1.26                     | 1.32              |
| 17:R:172:ARG:NH1  | 51:9:908:A:H5''   | 1.47                     | 1.29              |
| 48:5:2367:A:N1    | 48:5:2788:U:O4    | 1.66                     | 1.29              |
| 5:E:126:ARG:NH1   | 48:5:712:C:H1'    | 1.49                     | 1.27              |
| 61:JJ:121:LYS:CE  | 61:JJ:121:LYS:NZ  | 1.49                     | 1.26              |
| 51:9:872:A:N1     | 51:9:914:U:O4     | 1.72                     | 1.22              |
| 48:5:4213:A:N1    | 48:5:4218:U:O4    | 1.72                     | 1.21              |
| 48:5:1958:A:H5''  | 48:5:1962:A:O2'   | 1.03                     | 1.20              |
| 12:M:116:LYS:CG   | 14:O:196:LEU:HD21 | 1.72                     | 1.20              |
| 17:R:172:ARG:NH1  | 51:9:908:A:C5'    | 2.03                     | 1.20              |
| 48:5:1929:A:N1    | 48:5:2054:U:O4    | 1.75                     | 1.19              |
| 48:5:2468:U:O4    | 48:5:2473:A:N1    | 1.73                     | 1.19              |
| 5:E:202:VAL:HG13  | 5:E:256:LYS:NZ    | 1.55                     | 1.18              |
| 51:9:322:C:O2'    | 51:9:323:C:P      | 2.01                     | 1.17              |
| 9:I:191:ILE:CD1   | 9:I:200:ILE:HD12  | 1.74                     | 1.16              |
| 7:G:156:VAL:HG11  | 7:G:184:LEU:HD12  | 1.28                     | 1.14              |
| 5:E:59:TYR:CD2    | 5:E:64:LEU:HD12   | 1.83                     | 1.13              |
| 5:E:254:LEU:HD23  | 5:E:257:ILE:HD11  | 1.24                     | 1.13              |
| 17:R:172:ARG:HH11 | 51:9:908:A:H5''   | 0.98                     | 1.13              |
| 51:9:1137:U:C4    | 51:9:1148:A:N1    | 2.18                     | 1.12              |
| 9:I:191:ILE:HD11  | 9:I:200:ILE:HD12  | 1.29                     | 1.12              |
| 48:5:1958:A:C5'   | 48:5:1962:A:O2'   | 1.95                     | 1.11              |
| 11:L:163:LYS:HE2  | 48:5:509:A:H4'    | 1.16                     | 1.11              |
| 12:M:116:LYS:HG3  | 14:O:196:LEU:HD21 | 1.33                     | 1.09              |
| 5:E:126:ARG:HH11  | 48:5:712:C:C1'    | 1.65                     | 1.09              |
| 5:E:126:ARG:NH1   | 48:5:712:C:C1'    | 2.14                     | 1.08              |
| 9:I:191:ILE:HD12  | 9:I:200:ILE:CD1   | 1.84                     | 1.07              |
| 5:E:202:VAL:CG1   | 5:E:256:LYS:NZ    | 2.17                     | 1.07              |
| 9:I:191:ILE:CD1   | 9:I:200:ILE:CD1   | 2.33                     | 1.07              |
| 11:L:42:ARG:NH1   | 11:L:51:ALA:O     | 1.88                     | 1.06              |
| 5:E:62:LYS:NZ     | 48:5:978:G:OP2    | 1.88                     | 1.06              |
| 5:E:202:VAL:CG1   | 5:E:256:LYS:HZ2   | 1.68                     | 1.05              |
| 48:5:2409:U:C4    | 48:5:2783:A:N1    | 2.25                     | 1.05              |
| 47:3:67:U:C2'     | 47:3:68:C:H5'     | 1.86                     | 1.04              |
| 5:E:62:LYS:HE3    | 48:5:978:G:OP1    | 1.54                     | 1.04              |
| 5:E:202:VAL:HG13  | 5:E:256:LYS:HZ2   | 1.05                     | 1.04              |
| 47:3:41:U:O3'     | 57:FF:198:ARG:HD3 | 1.55                     | 1.04              |
| 51:9:322:C:O2'    | 51:9:323:C:O5'    | 1.73                     | 1.03              |
| 5:E:62:LYS:CE     | 48:5:978:G:P      | 2.46                     | 1.03              |
| 51:9:1307:U:C2'   | 51:9:1308:U:H5''  | 1.87                     | 1.03              |
| 51:9:872:A:N1     | 51:9:914:U:C4     | 2.27                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:9:1307:U:H2'   | 51:9:1308:U:H5''  | 1.04                     | 1.02              |
| 48:5:3751:G:C2'   | 48:5:3752:C:H5'   | 1.90                     | 1.02              |
| 5:E:126:ARG:HH11  | 48:5:712:C:H1'    | 0.92                     | 1.02              |
| 51:9:1137:U:O4    | 51:9:1148:A:C2    | 2.12                     | 1.01              |
| 48:5:1929:A:H61   | 48:5:2054:U:H3    | 1.10                     | 1.00              |
| 47:3:67:U:H2'     | 47:3:68:C:H5'     | 1.42                     | 1.00              |
| 9:I:202:ASN:O     | 49:7:63:C:C5      | 2.15                     | 0.99              |
| 5:E:126:ARG:NH1   | 48:5:712:C:C2'    | 2.26                     | 0.99              |
| 5:E:62:LYS:CE     | 48:5:978:G:OP2    | 2.10                     | 0.98              |
| 51:9:911:C:C2'    | 51:9:912:C:H5'    | 1.91                     | 0.98              |
| 47:3:41:U:O2'     | 57:FF:198:ARG:NH2 | 1.94                     | 0.98              |
| 10:J:80:GLU:OE2   | 10:J:170:TYR:OH   | 1.82                     | 0.98              |
| 48:5:77:U:O4      | 48:5:335:A:N1     | 1.98                     | 0.97              |
| 48:5:1968:G:H1    | 48:5:2018:C:H42   | 1.12                     | 0.97              |
| 48:5:3751:G:O2'   | 48:5:3752:C:H5'   | 1.65                     | 0.96              |
| 51:9:911:C:H2'    | 51:9:912:C:H5'    | 1.44                     | 0.96              |
| 2:B:163:LEU:HD21  | 2:B:182:GLU:CG    | 1.95                     | 0.96              |
| 48:5:1278:C:H3'   | 48:5:1279:A:H4'   | 1.48                     | 0.95              |
| 48:5:1983:A:N1    | 48:5:2008:U:C4    | 2.35                     | 0.95              |
| 48:5:4278:C:HO2'  | 48:5:4281:A:H8    | 1.06                     | 0.95              |
| 48:5:1983:A:N1    | 48:5:2008:U:O4    | 2.00                     | 0.95              |
| 48:5:957:G:H1'    | 48:5:958:G:OP2    | 1.67                     | 0.94              |
| 2:B:163:LEU:CD2   | 2:B:182:GLU:HG2   | 1.96                     | 0.94              |
| 5:E:126:ARG:HH12  | 48:5:712:C:C2'    | 1.81                     | 0.94              |
| 51:9:830:A:N6     | 51:9:844:U:N3     | 2.16                     | 0.94              |
| 17:R:172:ARG:HH12 | 51:9:908:A:H5'    | 1.29                     | 0.94              |
| 17:R:98:ARG:NH2   | 17:R:107:ARG:HH12 | 15.83                    | 0.94              |
| 51:9:830:A:N1     | 51:9:844:U:O4     | 2.01                     | 0.94              |
| 48:5:2409:U:O4    | 48:5:2783:A:N1    | 1.99                     | 0.93              |
| 51:9:1235:G:H5'   | 51:9:1247:C:H42   | 1.30                     | 0.93              |
| 51:9:1407:U:H2'   | 51:9:1408:U:C5    | 2.04                     | 0.92              |
| 17:R:98:ARG:HH22  | 17:R:107:ARG:HH12 | 16.44                    | 0.92              |
| 9:I:48:LEU:HD21   | 9:I:145:LYS:HG2   | 1.49                     | 0.92              |
| 5:E:126:ARG:NH1   | 48:5:712:C:O2'    | 2.03                     | 0.92              |
| 54:CC:63:VAL:O    | 54:CC:63:VAL:HG12 | 1.67                     | 0.92              |
| 48:5:976:G:C2'    | 48:5:977:C:O4'    | 2.17                     | 0.92              |
| 17:R:98:ARG:NH2   | 17:R:107:ARG:NH1  | 16.17                    | 0.92              |
| 2:B:163:LEU:CD2   | 2:B:182:GLU:CG    | 2.48                     | 0.92              |
| 12:M:116:LYS:HG2  | 14:O:196:LEU:HD21 | 1.49                     | 0.91              |
| 70:SS:11:HIS:O    | 70:SS:12:ILE:HD12 | 1.69                     | 0.91              |
| 48:5:2468:U:N3    | 48:5:2473:A:N6    | 2.17                     | 0.91              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:174:ARG:NH1    | 48:5:4985:U:O2    | 2.05                     | 0.90              |
| 48:5:1958:A:O2'    | 48:5:1959:U:H5''  | 1.72                     | 0.90              |
| 9:I:191:ILE:HD12   | 9:I:200:ILE:HD11  | 1.52                     | 0.90              |
| 5:E:251:SER:O      | 5:E:255:PRO:CD    | 2.20                     | 0.89              |
| 5:E:62:LYS:CE      | 48:5:978:G:OP1    | 2.20                     | 0.88              |
| 48:5:102:G:O2'     | 48:5:1381:U:O2'   | 1.90                     | 0.88              |
| 11:L:163:LYS:CE    | 48:5:509:A:H4'    | 2.04                     | 0.88              |
| 54:CC:73:VAL:HG12  | 54:CC:73:VAL:O    | 1.73                     | 0.87              |
| 48:5:1279:A:H3'    | 48:5:1280:C:H5''  | 1.57                     | 0.87              |
| 51:9:1455:A:O2'    | 51:9:1456:G:O5'   | 1.91                     | 0.87              |
| 2:B:156:TYR:CD1    | 48:5:4909:A:H2'   | 2.10                     | 0.86              |
| 51:9:872:A:C2      | 51:9:914:U:O4     | 2.26                     | 0.86              |
| 48:5:2027:U:O2'    | 48:5:2028:C:H5'   | 1.75                     | 0.86              |
| 9:I:49:CYS:SG      | 9:I:51:HIS:NE2    | 2.48                     | 0.86              |
| 5:E:238:ILE:O      | 5:E:239:THR:OG1   | 1.93                     | 0.85              |
| 5:E:62:LYS:HE2     | 48:5:978:G:OP2    | 1.76                     | 0.85              |
| 5:E:62:LYS:HE2     | 48:5:978:G:P      | 2.15                     | 0.85              |
| 51:9:1267:C:O2'    | 51:9:1268:C:H5'   | 1.76                     | 0.85              |
| 5:E:254:LEU:CD2    | 5:E:257:ILE:HD11  | 2.05                     | 0.85              |
| 9:I:184:MET:HE2    | 9:I:190:LEU:HG    | 1.57                     | 0.85              |
| 48:5:1279:A:C3'    | 48:5:1280:C:H5''  | 2.07                     | 0.85              |
| 48:5:1956:A:O2'    | 48:5:1957:U:H5'   | 1.77                     | 0.84              |
| 7:G:156:VAL:HG11   | 7:G:184:LEU:CD1   | 2.05                     | 0.84              |
| 17:R:172:ARG:NH1   | 51:9:908:A:H5'    | 1.89                     | 0.84              |
| 48:5:1957:U:O2'    | 48:5:1958:A:C8    | 2.29                     | 0.84              |
| 47:3:68:C:O2'      | 47:3:69:G:O4'     | 1.95                     | 0.84              |
| 54:CC:192:LEU:HD23 | 54:CC:227:TRP:NE1 | 1.93                     | 0.83              |
| 51:9:1385:G:O2'    | 51:9:1386:A:H5'   | 1.79                     | 0.83              |
| 51:9:872:A:C6      | 51:9:914:U:O4     | 2.30                     | 0.83              |
| 47:3:29:A:O2'      | 47:3:30:G:O5'     | 1.97                     | 0.83              |
| 4:D:33:ARG:NH2     | 49:7:7:G:O3'      | 2.10                     | 0.82              |
| 48:5:3629:A:H4'    | 51:9:1721:U:O2    | 1.80                     | 0.82              |
| 7:G:86:VAL:HG21    | 7:G:185:LYS:HE3   | 1.62                     | 0.82              |
| 51:9:1406:G:H3'    | 51:9:1407:U:H4'   | 1.62                     | 0.82              |
| 9:I:202:ASN:O      | 49:7:63:C:C4      | 2.32                     | 0.81              |
| 5:E:157:ARG:O      | 5:E:178:ASN:ND2   | 2.13                     | 0.81              |
| 7:G:87:LEU:HD23    | 7:G:184:LEU:CD2   | 2.10                     | 0.81              |
| 54:CC:211:LYS:O    | 54:CC:215:LEU:HG  | 1.80                     | 0.81              |
| 51:9:1681:U:O2'    | 51:9:1682:C:O4'   | 1.98                     | 0.81              |
| 47:3:67:U:C3'      | 47:3:68:C:H5'     | 2.10                     | 0.81              |
| 48:5:1367:C:C2     | 48:5:1370:G:H2'   | 2.15                     | 0.81              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:M:81:ASP:OD1    | 12:M:84:THR:HG23  | 1.80                     | 0.81              |
| 48:5:1379:C:H4'    | 48:5:1380:G:O4'   | 1.81                     | 0.81              |
| 15:P:127:ARG:NH2   | 48:5:2422:C:OP1   | 2.14                     | 0.81              |
| 2:B:163:LEU:HD21   | 2:B:182:GLU:HG3   | 1.61                     | 0.80              |
| 51:9:1420:G:HO2'   | 71:TT:4:VAL:N     | 1.79                     | 0.80              |
| 54:CC:192:LEU:HD23 | 54:CC:227:TRP:CD1 | 2.16                     | 0.80              |
| 51:9:523:A:OP2     | 61:JJ:38:ARG:HD3  | 1.81                     | 0.80              |
| 5:E:251:SER:O      | 5:E:255:PRO:HD2   | 1.81                     | 0.80              |
| 2:B:156:TYR:CE1    | 48:5:4909:A:H2'   | 2.17                     | 0.80              |
| 7:G:86:VAL:HG12    | 7:G:87:LEU:N      | 1.96                     | 0.80              |
| 2:B:163:LEU:HD23   | 2:B:182:GLU:HG2   | 1.64                     | 0.79              |
| 48:5:919:C:N4      | 48:5:920:C:C4     | 2.51                     | 0.79              |
| 48:5:745:G:H2'     | 48:5:746:A:O4'    | 1.82                     | 0.79              |
| 48:5:957:G:N2      | 48:5:959:G:O6     | 2.15                     | 0.79              |
| 48:5:4723:A:H2'    | 48:5:4724:A:C8    | 2.17                     | 0.79              |
| 51:9:292:A:O2'     | 51:9:293:C:OP2    | 2.01                     | 0.79              |
| 48:5:2395:A:O2'    | 48:5:2806:A:H1'   | 1.82                     | 0.79              |
| 7:G:87:LEU:HD23    | 7:G:184:LEU:HD21  | 1.64                     | 0.79              |
| 48:5:3629:A:C4'    | 51:9:1721:U:O2    | 2.30                     | 0.79              |
| 51:9:1144:A:H2'    | 51:9:1145:A:C8    | 2.17                     | 0.79              |
| 17:R:172:ARG:HH11  | 51:9:908:A:C5'    | 1.77                     | 0.79              |
| 48:5:1958:A:H5''   | 48:5:1962:A:HO2'  | 0.98                     | 0.79              |
| 48:5:1929:A:N6     | 48:5:2054:U:H3    | 1.80                     | 0.78              |
| 48:5:3751:G:H2'    | 48:5:3752:C:H5'   | 1.65                     | 0.78              |
| 48:5:2026:A:C2'    | 48:5:2027:U:H5'   | 2.14                     | 0.78              |
| 50:8:55:U:O4       | 50:8:62:A:N1      | 2.16                     | 0.78              |
| 2:B:163:LEU:HD21   | 2:B:182:GLU:HG2   | 1.59                     | 0.78              |
| 48:5:504:G:N1      | 48:5:654:C:C2     | 2.52                     | 0.78              |
| 48:5:1213:G:C6     | 48:5:1215:C:C2    | 2.71                     | 0.78              |
| 51:9:1454:A:OP1    | 69:RR:3:ARG:NE    | 2.16                     | 0.77              |
| 48:5:77:U:N3       | 48:5:335:A:N6     | 2.32                     | 0.77              |
| 48:5:1563:A:C8     | 51:9:678:U:H4'    | 2.19                     | 0.77              |
| 48:5:2769:U:C2     | 48:5:2770:C:C5    | 2.72                     | 0.77              |
| 48:5:3723:A:H2'    | 48:5:3724:A:C8    | 2.20                     | 0.77              |
| 51:9:1137:U:O4     | 51:9:1148:A:C6    | 2.37                     | 0.77              |
| 5:E:202:VAL:CG1    | 5:E:256:LYS:HZ1   | 1.97                     | 0.76              |
| 48:5:2793:G:C6     | 48:5:2797:C:C4    | 2.74                     | 0.76              |
| 51:9:1235:G:H5'    | 51:9:1247:C:N4    | 2.00                     | 0.76              |
| 2:B:36:ASP:OD2     | 2:B:39:LYS:HE2    | 1.83                     | 0.76              |
| 9:I:184:MET:HE1    | 9:I:190:LEU:HD11  | 1.67                     | 0.76              |
| 48:5:2468:U:C4     | 48:5:2473:A:N1    | 2.54                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 51:9:1268:C:O2'  | 51:9:1269:G:O5'   | 2.04                     | 0.76              |
| 51:9:945:U:H2'   | 51:9:946:U:C6     | 2.21                     | 0.75              |
| 47:3:35:U:C1'    | 51:9:1641:A:OP1   | 2.34                     | 0.75              |
| 9:I:184:MET:CE   | 9:I:190:LEU:CD1   | 2.64                     | 0.75              |
| 51:9:643:A:OP2   | 61:JJ:38:ARG:NH2  | 2.19                     | 0.75              |
| 4:D:35:ARG:HB2   | 48:5:4325:A:C2    | 2.21                     | 0.75              |
| 63:LL:131:CYS:SG | 63:LL:132:ARG:N   | 2.60                     | 0.75              |
| 48:5:2779:C:O2'  | 50:8:112:G:OP1    | 2.05                     | 0.75              |
| 51:9:1102:G:N2   | 51:9:1103:C:C2    | 2.54                     | 0.75              |
| 45:1:57:ARG:NH2  | 48:5:3862:A:O2'   | 2.20                     | 0.74              |
| 74:WW:6:VAL:HG12 | 74:WW:34:ILE:HD11 | 1.69                     | 0.74              |
| 51:9:1307:U:H2'  | 51:9:1308:U:C5'   | 2.01                     | 0.74              |
| 51:9:1407:U:H2'  | 51:9:1408:U:C6    | 2.22                     | 0.74              |
| 9:I:184:MET:CE   | 9:I:190:LEU:HG    | 2.16                     | 0.74              |
| 3:C:158:VAL:HA   | 3:C:161:TYR:CE2   | 2.22                     | 0.74              |
| 3:C:159:GLU:OE1  | 3:C:159:GLU:N     | 2.20                     | 0.74              |
| 48:5:504:G:C2    | 48:5:654:C:O2     | 2.39                     | 0.74              |
| 4:D:200:MET:HE1  | 4:D:241:LYS:CG    | 2.17                     | 0.74              |
| 9:I:191:ILE:HD11 | 9:I:200:ILE:CD1   | 2.08                     | 0.74              |
| 51:9:1405:A:H2'  | 51:9:1406:G:O4'   | 1.88                     | 0.74              |
| 51:9:1680:G:O2'  | 51:9:1681:U:H5'   | 1.88                     | 0.74              |
| 51:9:872:A:C6    | 51:9:914:U:C4     | 2.75                     | 0.74              |
| 7:G:86:VAL:HG11  | 7:G:185:LYS:HG2   | 1.68                     | 0.74              |
| 48:5:4371:G:O2'  | 48:5:4372:U:OP2   | 2.05                     | 0.74              |
| 48:5:1279:A:H3'  | 48:5:1280:C:C5'   | 2.18                     | 0.74              |
| 48:5:22:G:N2     | 50:8:35:C:C2      | 2.56                     | 0.73              |
| 48:5:1278:C:C3'  | 48:5:1279:A:H4'   | 2.18                     | 0.73              |
| 11:L:116:ARG:NH1 | 11:L:155:MET:O    | 2.21                     | 0.73              |
| 48:5:3914:U:H3   | 48:5:4378:A:N6    | 1.86                     | 0.73              |
| 48:5:956:A:H4'   | 48:5:957:G:OP2    | 1.89                     | 0.73              |
| 51:9:1386:A:O2'  | 51:9:1387:G:H5'   | 1.89                     | 0.72              |
| 47:3:76:A:N7     | 48:5:4371:G:C6    | 2.58                     | 0.72              |
| 48:5:1280:C:C4   | 48:5:1282:G:C6    | 2.77                     | 0.72              |
| 3:C:157:LYS:O    | 3:C:160:GLY:N     | 2.20                     | 0.72              |
| 5:E:62:LYS:HE3   | 48:5:978:G:P      | 2.20                     | 0.72              |
| 5:E:254:LEU:HD22 | 5:E:258:LYS:HE3   | 1.72                     | 0.72              |
| 7:G:86:VAL:HG12  | 7:G:87:LEU:H      | 1.55                     | 0.71              |
| 56:EE:154:ILE:O  | 56:EE:155:LYS:HG3 | 1.89                     | 0.71              |
| 48:5:2367:A:N1   | 48:5:2788:U:C4    | 2.57                     | 0.71              |
| 51:9:65:C:N4     | 58:GG:134:GLY:O   | 2.24                     | 0.71              |
| 48:5:977:C:C2'   | 48:5:978:G:H5'    | 2.20                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:2367:A:N6    | 48:5:2788:U:H3     | 1.88                     | 0.71              |
| 48:5:1958:A:H4'   | 48:5:1962:A:H1'    | 1.72                     | 0.71              |
| 48:5:2632:U:H2'   | 48:5:2633:U:C6     | 2.25                     | 0.71              |
| 5:E:251:SER:O     | 5:E:255:PRO:HD3    | 1.91                     | 0.71              |
| 48:5:3752:C:O2'   | 48:5:3753:G:OP2    | 2.09                     | 0.71              |
| 48:5:2026:A:O2'   | 48:5:2027:U:H5'    | 1.90                     | 0.71              |
| 48:5:516:C:C2     | 48:5:646:G:N2      | 2.59                     | 0.71              |
| 51:9:1444:U:H2'   | 51:9:1445:U:C6     | 2.26                     | 0.71              |
| 7:G:86:VAL:CG1    | 7:G:87:LEU:H       | 2.04                     | 0.71              |
| 54:CC:192:LEU:HB3 | 54:CC:227:TRP:CD1  | 2.26                     | 0.71              |
| 48:5:723:A:C2     | 48:5:943:A:N1      | 2.59                     | 0.71              |
| 48:5:977:C:C2     | 48:5:978:G:C8      | 2.79                     | 0.71              |
| 51:9:1235:G:H2'   | 51:9:1236:G:C8     | 2.26                     | 0.71              |
| 48:5:1724:G:H4'   | 48:5:1725:U:OP2    | 1.89                     | 0.71              |
| 5:E:217:GLN:NE2   | 5:E:233:LYS:HD2    | 2.05                     | 0.71              |
| 48:5:181:C:N3     | 48:5:256:G:C2      | 2.59                     | 0.70              |
| 7:G:87:LEU:CD2    | 7:G:184:LEU:HD21   | 2.20                     | 0.70              |
| 47:3:39:U:O4'     | 57:FF:135:ARG:NH2  | 2.23                     | 0.70              |
| 9:I:87:ILE:HG12   | 9:I:138:ILE:HG12   | 1.74                     | 0.70              |
| 48:5:499:G:N2     | 48:5:656:C:C2      | 2.60                     | 0.70              |
| 51:9:751:G:C2     | 51:9:792:C:N3      | 2.59                     | 0.70              |
| 51:9:1455:A:HO2'  | 51:9:1456:G:P      | 2.15                     | 0.70              |
| 48:5:1958:A:C5'   | 48:5:1962:A:HO2'   | 1.88                     | 0.70              |
| 51:9:1212:G:O2'   | 51:9:1213:C:O5'    | 2.10                     | 0.70              |
| 48:5:4901:G:N2    | 48:5:4921:C:C2     | 2.60                     | 0.69              |
| 48:5:482:G:H2'    | 48:5:483:G:C8      | 2.27                     | 0.69              |
| 57:FF:35:LEU:HD23 | 57:FF:147:VAL:HG22 | 1.73                     | 0.69              |
| 54:CC:63:VAL:CG1  | 54:CC:63:VAL:O     | 2.41                     | 0.69              |
| 48:5:2773:G:N2    | 48:5:2774:C:C2     | 2.61                     | 0.69              |
| 48:5:4510:A:O2'   | 48:5:4511:A:O4'    | 2.11                     | 0.69              |
| 48:5:1968:G:H1    | 48:5:2018:C:N4     | 1.89                     | 0.69              |
| 48:5:1279:A:C2'   | 48:5:1280:C:H5''   | 2.21                     | 0.69              |
| 9:I:187:GLU:OE1   | 9:I:189:ARG:NE     | 2.24                     | 0.69              |
| 2:B:163:LEU:CD2   | 2:B:182:GLU:HG3    | 2.17                     | 0.69              |
| 48:5:166:C:O2     | 48:5:166:C:H2'     | 1.90                     | 0.69              |
| 48:5:4075:U:O2'   | 48:5:4076:G:H2'    | 1.91                     | 0.69              |
| 48:5:2367:A:N6    | 48:5:2788:U:N3     | 2.40                     | 0.69              |
| 48:5:4481:U:H2'   | 48:5:4482:U:C6     | 2.27                     | 0.69              |
| 7:G:156:VAL:CG1   | 7:G:184:LEU:HD12   | 2.14                     | 0.69              |
| 48:5:499:G:C2     | 48:5:656:C:C2      | 2.81                     | 0.69              |
| 4:D:69:ILE:HD11   | 19:T:28:ALA:HB1    | 1.75                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:309:G:N2     | 51:9:310:C:C2      | 2.61                     | 0.69              |
| 48:5:1635:C:H2'   | 48:5:1636:U:H5'    | 1.75                     | 0.69              |
| 48:5:1929:A:N1    | 48:5:2054:U:C4     | 2.59                     | 0.68              |
| 2:B:261:ARG:HE    | 48:5:3870:C:H4'    | 1.57                     | 0.68              |
| 48:5:1367:C:N3    | 48:5:1369:C:OP2    | 2.26                     | 0.68              |
| 48:5:978:G:H2'    | 48:5:979:C:O4'     | 1.92                     | 0.68              |
| 48:5:504:G:C6     | 48:5:654:C:N3      | 2.61                     | 0.68              |
| 48:5:166:C:O2     | 48:5:167:C:H5      | 1.76                     | 0.68              |
| 47:3:1:G:N2       | 47:3:2:C:C2        | 2.61                     | 0.68              |
| 51:9:289:G:OP1    | 56:EE:155:LYS:HE3  | 1.94                     | 0.68              |
| 47:3:13:C:N3      | 47:3:22:G:O6       | 2.26                     | 0.68              |
| 48:5:1991:A:N6    | 48:5:2003:G:OP1    | 2.25                     | 0.68              |
| 48:5:1958:A:O2'   | 48:5:1959:U:C5'    | 2.41                     | 0.68              |
| 48:5:1380:G:O2'   | 48:5:1381:U:O2     | 2.10                     | 0.68              |
| 47:3:39:U:O2'     | 47:3:40:C:H6       | 1.77                     | 0.68              |
| 66:OO:95:ILE:HD11 | 66:OO:126:ILE:HD12 | 1.75                     | 0.68              |
| 47:3:76:A:N6      | 48:5:4371:G:N7     | 2.41                     | 0.68              |
| 51:9:1235:G:H2'   | 51:9:1236:G:H8     | 1.59                     | 0.68              |
| 47:3:76:A:C6      | 48:5:4371:G:C5     | 2.81                     | 0.68              |
| 51:9:1253:A:OP2   | 51:9:1526:G:N2     | 2.26                     | 0.68              |
| 51:9:1406:G:C3'   | 51:9:1407:U:H4'    | 2.24                     | 0.67              |
| 3:C:313:VAL:HG11  | 6:F:172:THR:HG21   | 1.76                     | 0.67              |
| 48:5:497:G:N2     | 48:5:657:C:C2      | 2.62                     | 0.67              |
| 48:5:2409:U:C4    | 48:5:2783:A:C2     | 2.82                     | 0.67              |
| 48:5:642:G:N2     | 48:5:643:C:C2      | 2.62                     | 0.67              |
| 48:5:4453:C:C2    | 48:5:4529:G:C2     | 2.82                     | 0.67              |
| 51:9:1109:C:O2    | 51:9:1109:C:H2'    | 1.93                     | 0.67              |
| 48:5:2288:G:N2    | 48:5:2290:C:C2     | 2.63                     | 0.67              |
| 51:9:1137:U:N3    | 51:9:1148:A:N6     | 2.42                     | 0.67              |
| 58:GG:67:VAL:HG23 | 58:GG:99:GLY:HA2   | 1.74                     | 0.67              |
| 51:9:1137:U:C4    | 51:9:1148:A:C6     | 2.82                     | 0.67              |
| 48:5:1358:G:H8    | 48:5:1358:G:H3'    | 1.58                     | 0.67              |
| 48:5:3914:U:H3    | 48:5:4378:A:H61    | 1.37                     | 0.67              |
| 48:5:166:C:O2     | 48:5:167:C:C5      | 2.48                     | 0.67              |
| 6:F:245:LEU:HD23  | 6:F:249:MET:HG3    | 1.77                     | 0.67              |
| 48:5:973:G:N2     | 48:5:1282:G:O2'    | 2.28                     | 0.67              |
| 3:C:210:ILE:HG21  | 3:C:252:TRP:CZ3    | 2.30                     | 0.67              |
| 47:3:39:U:H4'     | 66:OO:66:ARG:HH22  | 1.60                     | 0.67              |
| 48:5:5026:U:OP2   | 60:II:79:ILE:HD13  | 1.95                     | 0.67              |
| 51:9:1447:G:H2'   | 51:9:1448:A:C8     | 2.30                     | 0.67              |
| 48:5:1268:G:H4'   | 48:5:1269:G:OP1    | 1.95                     | 0.67              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 51:9:446:G:OP2   | 60:II:47:ARG:NH1   | 2.27                     | 0.67              |
| 48:5:1264:C:H2'  | 48:5:1265:G:O4'    | 1.95                     | 0.67              |
| 11:L:56:ARG:O    | 11:L:116:ARG:NH2   | 2.28                     | 0.66              |
| 5:E:161:LEU:HD21 | 5:E:253:ILE:HD11   | 1.76                     | 0.66              |
| 48:5:1957:U:O2'  | 48:5:1958:A:H8     | 1.78                     | 0.66              |
| 48:5:1359:G:H2'  | 48:5:1360:G:C8     | 2.30                     | 0.66              |
| 10:J:83:LEU:HD12 | 10:J:170:TYR:OH    | 1.96                     | 0.66              |
| 48:5:22:G:C2     | 50:8:35:C:N3       | 2.64                     | 0.66              |
| 51:9:1466:G:N2   | 51:9:1467:C:C2     | 2.63                     | 0.66              |
| 51:9:103:A:OP2   | 51:9:356:C:N4      | 2.29                     | 0.66              |
| 48:5:1957:U:C2'  | 48:5:1958:A:C8     | 2.79                     | 0.66              |
| 25:Z:52:LYS:O    | 25:Z:65:ARG:NH2    | 2.29                     | 0.66              |
| 47:3:33:U:P      | 57:FF:127:ARG:HH12 | 2.19                     | 0.66              |
| 51:9:1308:U:H2'  | 51:9:1309:C:O4'    | 1.96                     | 0.66              |
| 10:J:83:LEU:HD12 | 10:J:170:TYR:CZ    | 2.31                     | 0.66              |
| 48:5:2826:U:H4'  | 48:5:2827:G:H5'    | 1.77                     | 0.66              |
| 48:5:1358:G:C6   | 48:5:1379:C:N3     | 2.64                     | 0.66              |
| 51:9:316:G:N2    | 51:9:317:C:C2      | 2.64                     | 0.66              |
| 48:5:199:G:C6    | 48:5:201:C:N4      | 2.64                     | 0.66              |
| 5:E:202:VAL:HG13 | 5:E:256:LYS:HZ1    | 1.50                     | 0.65              |
| 76:YY:110:ARG:O  | 76:YY:113:ARG:O    | 2.14                     | 0.65              |
| 51:9:1526:G:N2   | 51:9:1527:C:C2     | 2.65                     | 0.65              |
| 51:9:15:U:H2'    | 51:9:16:G:O4'      | 1.95                     | 0.65              |
| 71:TT:38:LYS:O   | 71:TT:39:LEU:HB2   | 1.95                     | 0.65              |
| 48:5:1958:A:H3'  | 48:5:1958:A:OP2    | 1.96                     | 0.65              |
| 9:I:184:MET:HG2  | 9:I:189:ARG:HD2    | 1.79                     | 0.65              |
| 4:D:23:ARG:NH2   | 48:5:4280:A:OP2    | 2.29                     | 0.65              |
| 48:5:723:A:H2    | 48:5:943:A:N1      | 1.93                     | 0.65              |
| 51:9:1727:G:H2'  | 51:9:1728:U:O4'    | 1.97                     | 0.65              |
| 48:5:1635:C:C2'  | 48:5:1636:U:H5'    | 2.27                     | 0.65              |
| 51:9:1679:A:O2'  | 51:9:1680:G:OP2    | 2.09                     | 0.65              |
| 3:C:271:ALA:O    | 3:C:272:SER:OG     | 2.11                     | 0.65              |
| 47:3:39:U:O2'    | 47:3:40:C:O5'      | 2.14                     | 0.65              |
| 2:B:14:LEU:HD23  | 2:B:17:LEU:HD21    | 1.77                     | 0.65              |
| 48:5:1378:C:H3'  | 48:5:1379:C:C5'    | 2.26                     | 0.65              |
| 4:D:200:MET:CE   | 4:D:241:LYS:HE3    | 2.26                     | 0.65              |
| 2:B:45:ALA:HB3   | 2:B:183:ILE:HG23   | 1.79                     | 0.65              |
| 48:5:1969:G:O2'  | 48:5:1970:A:H5'    | 1.97                     | 0.65              |
| 51:9:164:A:O2'   | 51:9:165:G:O4'     | 2.15                     | 0.65              |
| 2:B:254:ILE:HG23 | 2:B:266:VAL:HG11   | 1.78                     | 0.65              |
| 51:9:1102:G:N1   | 51:9:1103:C:C4     | 2.65                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:9:1681:U:O2'   | 51:9:1682:C:O5'   | 2.14                     | 0.64              |
| 51:9:1416:C:H2'   | 51:9:1417:C:C2    | 2.33                     | 0.64              |
| 51:9:980:A:H2'    | 51:9:981:A:C8     | 2.32                     | 0.64              |
| 51:9:200:G:N2     | 51:9:201:C:C2     | 2.65                     | 0.64              |
| 48:5:2468:U:H3    | 48:5:2473:A:N6    | 1.91                     | 0.64              |
| 9:I:191:ILE:CD1   | 9:I:200:ILE:HD11  | 2.14                     | 0.64              |
| 48:5:1358:G:C8    | 48:5:1358:G:H3'   | 2.32                     | 0.64              |
| 51:9:1401:A:C2    | 51:9:1402:A:C6    | 2.85                     | 0.64              |
| 48:5:2258:C:H2'   | 48:5:2258:C:O2    | 1.96                     | 0.64              |
| 9:I:184:MET:CE    | 9:I:190:LEU:HD11  | 2.27                     | 0.64              |
| 48:5:2090:U:P     | 48:5:2090:U:O4'   | 2.56                     | 0.64              |
| 51:9:522:A:O3'    | 61:JJ:131:ARG:NH2 | 2.31                     | 0.64              |
| 48:5:1404:G:C2    | 48:5:1414:C:C2    | 2.85                     | 0.64              |
| 68:QQ:12:VAL:HG21 | 68:QQ:91:ALA:HA   | 1.80                     | 0.64              |
| 51:9:50:A:N1      | 51:9:488:U:O4     | 2.30                     | 0.64              |
| 14:O:201:PHE:HB2  | 14:O:202:LEU:HD13 | 1.80                     | 0.64              |
| 51:9:1617:G:N7    | 67:PP:43:ARG:NH1  | 2.46                     | 0.64              |
| 48:5:986:C:C2     | 48:5:1068:G:N2    | 2.65                     | 0.64              |
| 49:7:30:C:C2      | 49:7:48:G:N2      | 2.65                     | 0.64              |
| 48:5:5066:U:H2'   | 48:5:5067:U:C6    | 2.32                     | 0.64              |
| 48:5:2084:C:H3'   | 48:5:2085:G:C5'   | 2.27                     | 0.64              |
| 56:EE:31:PRO:CD   | 56:EE:38:LEU:HD13 | 2.28                     | 0.64              |
| 51:9:1835:A:C4    | 51:9:1863:A:N7    | 2.66                     | 0.64              |
| 9:I:184:MET:HE1   | 9:I:190:LEU:CD1   | 2.27                     | 0.64              |
| 51:9:1384:C:C2'   | 51:9:1385:G:H5'   | 2.28                     | 0.64              |
| 51:9:1211:G:O2'   | 51:9:1212:G:H5'   | 1.97                     | 0.64              |
| 48:5:1682:A:C2    | 48:5:1683:U:C2    | 2.85                     | 0.64              |
| 56:EE:163:ASP:O   | 56:EE:164:LEU:HB2 | 1.97                     | 0.64              |
| 48:5:2268:A:H4'   | 48:5:2269:C:H5'   | 1.80                     | 0.64              |
| 7:G:86:VAL:HG13   | 7:G:183:ILE:O     | 1.98                     | 0.63              |
| 48:5:969:C:O2'    | 48:5:970:G:N3     | 2.31                     | 0.63              |
| 51:9:200:G:N1     | 51:9:201:C:C4     | 2.66                     | 0.63              |
| 51:9:1859:A:C2    | 51:9:1860:A:C6    | 2.85                     | 0.63              |
| 71:TT:33:TRP:O    | 71:TT:35:ASP:N    | 2.31                     | 0.63              |
| 48:5:4213:A:N1    | 48:5:4218:U:C4    | 2.61                     | 0.63              |
| 48:5:4723:A:C2    | 48:5:4724:A:C6    | 2.86                     | 0.63              |
| 48:5:1213:G:N1    | 48:5:1215:C:C2    | 2.67                     | 0.63              |
| 48:5:4579:U:H2'   | 48:5:4580:U:C6    | 2.33                     | 0.63              |
| 48:5:1378:C:H3'   | 48:5:1379:C:H5'   | 1.81                     | 0.63              |
| 4:D:200:MET:HE1   | 4:D:241:LYS:HG3   | 1.80                     | 0.63              |
| 48:5:167:C:C2     | 48:5:269:G:N2     | 2.66                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 48:5:1823:G:O3'  | 48:5:1825:A:P     | 2.56                     | 0.63              |
| 51:9:107:A:H2'   | 51:9:108:G:C8     | 2.33                     | 0.63              |
| 48:5:976:G:H4'   | 48:5:976:G:OP1    | 1.98                     | 0.63              |
| 4:D:200:MET:HE2  | 4:D:241:LYS:HE3   | 1.80                     | 0.63              |
| 47:3:41:U:O3'    | 57:FF:198:ARG:CD  | 2.40                     | 0.63              |
| 54:CC:73:VAL:CG1 | 54:CC:73:VAL:O    | 2.47                     | 0.63              |
| 47:3:37:A:C2'    | 47:3:38:A:H5'     | 2.28                     | 0.63              |
| 17:R:107:ARG:C   | 17:R:107:ARG:HD2  | 3.55                     | 0.63              |
| 5:E:254:LEU:HD23 | 5:E:257:ILE:CD1   | 2.14                     | 0.63              |
| 48:5:1550:G:C2   | 48:5:1579:C:C2    | 2.86                     | 0.63              |
| 51:9:830:A:N6    | 51:9:844:U:H3     | 1.97                     | 0.63              |
| 9:I:184:MET:HE2  | 9:I:190:LEU:CG    | 2.27                     | 0.63              |
| 48:5:504:G:C6    | 48:5:654:C:C2     | 2.87                     | 0.63              |
| 6:F:161:TYR:CE2  | 6:F:170:ALA:HB2   | 2.34                     | 0.63              |
| 48:5:22:G:C2     | 50:8:35:C:C2      | 2.87                     | 0.62              |
| 11:L:65:ARG:HG2  | 11:L:66:TYR:CE2   | 2.34                     | 0.62              |
| 48:5:1983:A:C6   | 48:5:2008:U:O4    | 2.52                     | 0.62              |
| 47:3:35:U:H1'    | 51:9:1641:A:OP1   | 1.98                     | 0.62              |
| 3:C:158:VAL:HA   | 3:C:161:TYR:CD2   | 2.33                     | 0.62              |
| 9:I:204:GLY:O    | 9:I:205:PRO:O     | 2.16                     | 0.62              |
| 48:5:2547:G:N2   | 48:5:2548:C:C2    | 2.68                     | 0.62              |
| 51:9:1842:C:C2   | 51:9:1858:G:C2    | 2.87                     | 0.62              |
| 51:9:1211:G:C2'  | 51:9:1212:G:H5'   | 2.29                     | 0.62              |
| 48:5:1879:C:O2'  | 48:5:1891:A:N3    | 2.29                     | 0.62              |
| 48:5:3668:C:C2   | 48:5:3675:G:C2    | 2.87                     | 0.62              |
| 3:C:32:ILE:HD12  | 3:C:130:ALA:HB2   | 1.82                     | 0.62              |
| 48:5:2108:G:C6   | 48:5:2125:C:N4    | 2.67                     | 0.62              |
| 48:5:1339:U:H2'  | 48:5:1340:C:C6    | 2.34                     | 0.62              |
| 7:G:87:LEU:CD2   | 7:G:184:LEU:CD2   | 2.77                     | 0.62              |
| 48:5:3900:G:N2   | 48:5:4562:C:C2    | 2.67                     | 0.62              |
| 51:9:448:A:H5''  | 60:II:25:ARG:HA   | 1.80                     | 0.62              |
| 4:D:200:MET:CE   | 4:D:241:LYS:HG3   | 2.28                     | 0.62              |
| 7:G:86:VAL:CG1   | 7:G:87:LEU:N      | 2.57                     | 0.62              |
| 12:M:81:ASP:OD1  | 12:M:84:THR:CG2   | 2.47                     | 0.62              |
| 48:5:4769:G:H2'  | 48:5:4770:U:O4'   | 2.00                     | 0.62              |
| 48:5:3783:A:H4'  | 48:5:3784:A:H5''  | 1.81                     | 0.62              |
| 53:BB:30:TRP:CZ2 | 53:BB:48:LEU:HD23 | 2.35                     | 0.62              |
| 51:9:1408:U:O4   | 51:9:1409:A:N6    | 2.33                     | 0.62              |
| 48:5:2409:U:O4   | 48:5:2783:A:C6    | 2.52                     | 0.62              |
| 9:I:184:MET:CE   | 9:I:190:LEU:CG    | 2.78                     | 0.62              |
| 51:9:217:A:C2    | 51:9:309:G:N1     | 2.67                     | 0.62              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 48:5:3765:G:O2'  | 48:5:3766:A:C8     | 2.49                     | 0.62              |
| 48:5:3723:A:C2   | 48:5:3724:A:C6     | 2.88                     | 0.61              |
| 51:9:751:G:N2    | 51:9:792:C:C2      | 2.68                     | 0.61              |
| 51:9:33:G:O6     | 51:9:522:A:H2      | 1.83                     | 0.61              |
| 48:5:1081:C:C2   | 48:5:1220:G:C2     | 2.87                     | 0.61              |
| 48:5:2905:C:C2   | 48:5:3590:G:N2     | 2.68                     | 0.61              |
| 51:9:488:U:H2'   | 51:9:488:U:O2      | 2.00                     | 0.61              |
| 51:9:1771:G:N2   | 51:9:1772:C:C2     | 2.67                     | 0.61              |
| 24:Y:49:ILE:HD13 | 24:Y:80:ILE:HD13   | 1.82                     | 0.61              |
| 48:5:1241:C:N4   | 48:5:1270:A:O2'    | 2.34                     | 0.61              |
| 48:5:1296:G:H1'  | 48:5:1297:U:P      | 2.41                     | 0.61              |
| 16:Q:65:ARG:NH1  | 48:5:1502:G:OP1    | 2.32                     | 0.61              |
| 48:5:77:U:H3     | 48:5:335:A:N6      | 1.97                     | 0.61              |
| 48:5:2045:G:O6   | 48:5:3870:C:O2'    | 2.17                     | 0.61              |
| 48:5:1723:A:N1   | 48:5:1838:A:C2     | 2.67                     | 0.61              |
| 5:E:59:TYR:CD2   | 5:E:64:LEU:CD1     | 2.73                     | 0.61              |
| 48:5:1358:G:C8   | 48:5:1358:G:C3'    | 2.84                     | 0.61              |
| 51:9:1233:G:O2'  | 51:9:1234:C:H5'    | 1.99                     | 0.61              |
| 48:5:4885:U:H2'  | 48:5:4886:C:O4'    | 1.99                     | 0.61              |
| 51:9:834:C:N3    | 51:9:841:G:C2      | 2.68                     | 0.61              |
| 48:5:1186:U:H2'  | 48:5:1187:G:O4'    | 2.00                     | 0.61              |
| 48:5:1983:A:C2   | 48:5:2008:U:C4     | 2.87                     | 0.61              |
| 74:WW:6:VAL:HG13 | 74:WW:29:PRO:HG2   | 1.83                     | 0.61              |
| 51:9:1616:U:OP2  | 67:PP:43:ARG:NH2   | 2.33                     | 0.61              |
| 48:5:2127:C:H2'  | 48:5:2128:G:C8     | 2.36                     | 0.61              |
| 47:3:38:A:O2'    | 47:3:39:U:H5'      | 2.00                     | 0.61              |
| 48:5:2758:G:O2'  | 48:5:2764:A:N3     | 2.26                     | 0.61              |
| 48:5:1999:A:H1'  | 48:5:2017:A:N1     | 2.16                     | 0.61              |
| 48:5:977:C:C4    | 48:5:978:G:N7      | 2.69                     | 0.61              |
| 58:GG:3:LEU:HD13 | 58:GG:111:LEU:HD11 | 1.82                     | 0.61              |
| 18:S:9:GLU:HG2   | 18:S:33:PHE:CE2    | 2.36                     | 0.61              |
| 48:5:1957:U:C2'  | 48:5:1958:A:H8     | 2.14                     | 0.61              |
| 51:9:409:C:C2    | 51:9:432:G:N2      | 2.68                     | 0.61              |
| 48:5:2623:A:C2   | 48:5:2624:G:C5     | 2.89                     | 0.61              |
| 48:5:197:A:N1    | 48:5:225:G:O2'     | 2.25                     | 0.61              |
| 48:5:1987:C:H2'  | 48:5:1987:C:O2     | 2.00                     | 0.61              |
| 51:9:1351:G:O2'  | 51:9:1378:A:N1     | 2.20                     | 0.61              |
| 48:5:3594:C:O2   | 48:5:3594:C:H2'    | 2.01                     | 0.61              |
| 48:5:4411:G:C2   | 48:5:4432:C:C2     | 2.89                     | 0.61              |
| 48:5:2554:U:H4'  | 48:5:2555:G:OP1    | 2.01                     | 0.61              |
| 2:B:163:LEU:HD23 | 2:B:182:GLU:CG     | 2.24                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:LL:77:VAL:HG22  | 63:LL:86:ILE:HD12  | 1.83                     | 0.60              |
| 51:9:1531:A:H2'    | 51:9:1532:C:C6     | 2.36                     | 0.60              |
| 1:A:234:LYS:HG2    | 1:A:238:ILE:HD12   | 1.83                     | 0.60              |
| 48:5:181:C:C2      | 48:5:256:G:N2      | 2.69                     | 0.60              |
| 51:9:301:A:N3      | 60:II:73:THR:HG21  | 2.15                     | 0.60              |
| 2:B:120:LYS:N      | 48:5:4968:A:OP1    | 2.33                     | 0.60              |
| 48:5:111:C:C2      | 48:5:331:G:C2      | 2.89                     | 0.60              |
| 51:9:474:G:N2      | 51:9:475:C:C2      | 2.70                     | 0.60              |
| 3:C:114:ARG:HB2    | 3:C:114:ARG:CZ     | 2.31                     | 0.60              |
| 48:5:3629:A:O4'    | 51:9:1721:U:O2     | 2.19                     | 0.60              |
| 3:C:45:ARG:NH2     | 48:5:2295:C:O2'    | 2.34                     | 0.60              |
| 48:5:515:C:C2      | 48:5:647:G:C2      | 2.90                     | 0.60              |
| 65:NN:125:LEU:HD22 | 65:NN:129:TYR:CE2  | 2.36                     | 0.60              |
| 3:C:76:ILE:HG22    | 3:C:77:PRO:HD2     | 1.84                     | 0.60              |
| 48:5:1213:G:C2     | 48:5:1215:C:O2     | 2.54                     | 0.60              |
| 48:5:286:U:H2'     | 48:5:287:U:C6      | 2.37                     | 0.60              |
| 48:5:106:A:H1'     | 48:5:336:A:C8      | 2.36                     | 0.60              |
| 48:5:2288:G:N1     | 48:5:2290:C:C4     | 2.70                     | 0.60              |
| 48:5:1268:G:C2     | 48:5:1270:A:C8     | 2.90                     | 0.60              |
| 13:N:202:ARG:NH2   | 48:5:1372:A:OP1    | 2.34                     | 0.60              |
| 48:5:4207:C:C2     | 48:5:4226:G:C2     | 2.90                     | 0.60              |
| 48:5:1672:U:H2'    | 48:5:1673:U:C6     | 2.36                     | 0.60              |
| 56:EE:173:ILE:HD11 | 56:EE:235:TRP:CE3  | 2.36                     | 0.60              |
| 51:9:1130:G:C2     | 51:9:1131:G:C8     | 2.89                     | 0.60              |
| 75:XX:41:PHE:O     | 75:XX:43:GLY:N     | 2.34                     | 0.60              |
| 48:5:2616:C:C2     | 48:5:2722:G:C2     | 2.89                     | 0.60              |
| 48:5:4283:G:N2     | 48:5:4284:C:C2     | 2.70                     | 0.60              |
| 48:5:2793:G:C5     | 48:5:2797:C:N4     | 2.69                     | 0.60              |
| 63:LL:66:VAL:HG23  | 63:LL:131:CYS:SG   | 2.42                     | 0.60              |
| 48:5:1839:U:H2'    | 48:5:1840:G:O4'    | 2.00                     | 0.60              |
| 48:5:4901:G:C2     | 48:5:4921:C:N3     | 2.70                     | 0.60              |
| 51:9:293:C:O2      | 51:9:293:C:H2'     | 2.02                     | 0.60              |
| 56:EE:48:LEU:HD21  | 56:EE:70:ILE:HD11  | 1.84                     | 0.60              |
| 56:EE:183:VAL:HG11 | 56:EE:220:THR:HG21 | 1.82                     | 0.60              |
| 51:9:1551:U:H2'    | 51:9:1552:G:C8     | 2.37                     | 0.60              |
| 48:5:4892:A:N1     | 48:5:4927:G:O6     | 2.35                     | 0.59              |
| 48:5:5000:G:C2     | 48:5:5051:C:C2     | 2.89                     | 0.59              |
| 51:9:598:G:C2      | 51:9:639:C:C2      | 2.90                     | 0.59              |
| 51:9:824:C:C2      | 61:JJ:144:ILE:HD13 | 2.36                     | 0.59              |
| 48:5:4092:G:N2     | 48:5:4158:C:C2     | 2.70                     | 0.59              |
| 48:5:3617:G:O2'    | 48:5:3620:G:N7     | 2.35                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:KK:15:LEU:HD22 | 62:KK:49:MET:CE   | 2.32                     | 0.59              |
| 62:KK:15:LEU:HD22 | 62:KK:49:MET:HE3  | 1.84                     | 0.59              |
| 51:9:1528:G:N2    | 51:9:1529:C:C2    | 2.70                     | 0.59              |
| 46:2:53:G:C2      | 46:2:62:C:C2      | 2.90                     | 0.59              |
| 48:5:1074:G:N2    | 48:5:1075:G:C2    | 2.71                     | 0.59              |
| 48:5:2827:G:H2'   | 48:5:2827:G:N3    | 2.18                     | 0.59              |
| 73:VV:55:ILE:HD11 | 73:VV:69:ILE:HD11 | 1.83                     | 0.59              |
| 55:DD:64:ARG:NH2  | 62:KK:73:ASN:OD1  | 2.35                     | 0.59              |
| 48:5:166:C:O2     | 48:5:166:C:C2'    | 2.49                     | 0.59              |
| 9:I:204:GLY:O     | 9:I:205:PRO:C     | 2.41                     | 0.59              |
| 51:9:834:C:H3'    | 51:9:835:C:C4'    | 2.33                     | 0.59              |
| 2:B:154:LYS:HB2   | 2:B:154:LYS:NZ    | 2.18                     | 0.59              |
| 48:5:222:C:H2'    | 48:5:223:G:O4'    | 2.03                     | 0.59              |
| 12:M:116:LYS:HG3  | 14:O:196:LEU:CD2  | 2.20                     | 0.59              |
| 47:3:5:G:N2       | 47:3:6:G:C4       | 2.71                     | 0.59              |
| 18:S:53:LYS:NZ    | 49:7:74:A:O2'     | 2.35                     | 0.59              |
| 3:C:108:TRP:HZ2   | 11:L:19:GLN:HE21  | 1.51                     | 0.59              |
| 47:3:41:U:C3'     | 57:FF:198:ARG:HD3 | 2.32                     | 0.59              |
| 48:5:917:A:C2     | 48:5:919:C:C5     | 2.90                     | 0.59              |
| 48:5:1266:G:H5''  | 48:5:2112:G:C2    | 2.37                     | 0.59              |
| 48:5:3662:A:H61   | 48:5:3680:U:H3    | 1.48                     | 0.59              |
| 48:5:1541:C:C2    | 48:5:1619:G:C2    | 2.90                     | 0.59              |
| 16:Q:104:ARG:NH2  | 48:5:1353:G:N7    | 2.50                     | 0.59              |
| 49:7:30:C:N3      | 49:7:48:G:C2      | 2.71                     | 0.59              |
| 58:GG:188:LYS:HA  | 58:GG:191:ARG:HD3 | 1.85                     | 0.59              |
| 48:5:2446:C:C2    | 48:5:2515:G:C2    | 2.90                     | 0.59              |
| 51:9:190:G:O2'    | 51:9:209:A:N6     | 2.36                     | 0.59              |
| 48:5:1957:U:H2'   | 48:5:1958:A:C8    | 2.38                     | 0.59              |
| 48:5:113:A:H2'    | 48:5:114:G:O4'    | 2.03                     | 0.59              |
| 51:9:50:A:N1      | 51:9:488:U:C4     | 2.71                     | 0.59              |
| 3:C:357:ALA:O     | 3:C:361:LYS:HG3   | 2.03                     | 0.59              |
| 14:O:18:ARG:NH2   | 48:5:2057:A:OP1   | 2.36                     | 0.59              |
| 48:5:2084:C:H3'   | 48:5:2085:G:H5'   | 1.84                     | 0.58              |
| 61:JJ:53:ILE:HD13 | 61:JJ:81:LEU:HD21 | 1.85                     | 0.58              |
| 48:5:2654:C:C2    | 48:5:2681:G:N2    | 2.71                     | 0.58              |
| 74:WW:106:THR:HG1 | 74:WW:109:GLY:H   | 1.52                     | 0.58              |
| 51:9:1398:G:N2    | 51:9:1399:C:C2    | 2.71                     | 0.58              |
| 51:9:217:A:C2     | 51:9:218:U:C6     | 2.90                     | 0.58              |
| 48:5:4219:A:H2'   | 48:5:4220:A:C8    | 2.37                     | 0.58              |
| 48:5:976:G:C2     | 48:5:977:C:C2     | 2.92                     | 0.58              |
| 10:J:119:TYR:HE2  | 10:J:125:ILE:HD11 | 1.67                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:309:G:N1     | 51:9:310:C:C4      | 2.71                     | 0.58              |
| 48:5:4441:A:H8    | 48:5:4441:A:H5''   | 1.68                     | 0.58              |
| 47:3:10:G:N2      | 47:3:11:C:C2       | 2.71                     | 0.58              |
| 51:9:872:A:N6     | 51:9:914:U:C5      | 2.72                     | 0.58              |
| 48:5:1957:U:H2'   | 48:5:1958:A:H8     | 1.67                     | 0.58              |
| 48:5:919:C:C4     | 48:5:920:C:C5      | 2.92                     | 0.58              |
| 51:9:752:G:C6     | 51:9:790:C:N4      | 2.71                     | 0.58              |
| 58:GG:5:ILE:HD12  | 58:GG:16:ILE:HD13  | 1.86                     | 0.58              |
| 48:5:1074:G:C2    | 48:5:1238:A:C2     | 2.91                     | 0.58              |
| 47:3:53:G:C2      | 47:3:62:C:C2       | 2.92                     | 0.58              |
| 51:9:1488:C:O2'   | 51:9:1490:G:OP2    | 2.22                     | 0.58              |
| 48:5:1213:G:O6    | 48:5:1215:C:C4     | 2.57                     | 0.58              |
| 48:5:642:G:N1     | 48:5:643:C:C4      | 2.71                     | 0.58              |
| 75:XX:67:ARG:HG2  | 75:XX:115:ILE:HD12 | 1.85                     | 0.58              |
| 20:U:87:THR:HG23  | 20:U:102:VAL:HG21  | 1.85                     | 0.58              |
| 47:3:13:C:O2      | 47:3:22:G:N1       | 2.32                     | 0.58              |
| 48:5:300:A:C2     | 48:5:301:G:C5      | 2.92                     | 0.58              |
| 57:FF:72:LEU:HD22 | 57:FF:112:LEU:HD11 | 1.86                     | 0.58              |
| 51:9:412:G:N2     | 51:9:429:C:C2      | 2.72                     | 0.58              |
| 48:5:707:C:C2     | 48:5:1291:G:C2     | 2.92                     | 0.58              |
| 48:5:685:C:H2'    | 48:5:685:C:O2      | 2.04                     | 0.58              |
| 56:EE:55:ALA:HB2  | 56:EE:64:ILE:HD12  | 1.85                     | 0.58              |
| 48:5:4754:G:C2    | 48:5:4880:C:C2     | 2.92                     | 0.58              |
| 48:5:1279:A:C3'   | 48:5:1280:C:C5'    | 2.78                     | 0.58              |
| 56:EE:156:MET:O   | 56:EE:157:ASN:ND2  | 2.37                     | 0.58              |
| 17:R:10:LEU:O     | 17:R:14:VAL:HG23   | 2.03                     | 0.58              |
| 52:AA:38:ILE:HD11 | 52:AA:150:THR:HG22 | 1.86                     | 0.58              |
| 51:9:31:U:O2'     | 51:9:643:A:N1      | 2.33                     | 0.58              |
| 47:3:76:A:C6      | 48:5:4371:G:N7     | 2.72                     | 0.58              |
| 58:GG:52:ILE:HD11 | 58:GG:109:LEU:HD22 | 1.86                     | 0.58              |
| 48:5:4757:C:O4'   | 48:5:4757:C:O2     | 2.21                     | 0.58              |
| 1:A:104:VAL:CG1   | 1:A:146:THR:HG21   | 2.34                     | 0.58              |
| 48:5:1280:C:C2    | 48:5:1282:G:C5     | 2.93                     | 0.57              |
| 48:5:1358:G:H2'   | 48:5:1359:G:O4'    | 2.04                     | 0.57              |
| 51:9:1543:U:HO2'  | 68:QQ:77:HIS:HE2   | 1.52                     | 0.57              |
| 48:5:245:C:O4'    | 48:5:245:C:O2      | 2.22                     | 0.57              |
| 48:5:1959:U:H1'   | 48:5:1961:G:C1'    | 2.35                     | 0.57              |
| 5:E:202:VAL:HG12  | 5:E:256:LYS:NZ     | 2.17                     | 0.57              |
| 51:9:643:A:OP1    | 51:9:643:A:H4'     | 2.04                     | 0.57              |
| 48:5:5026:U:H3'   | 60:II:79:ILE:CD1   | 2.34                     | 0.57              |
| 48:5:1840:G:H3'   | 48:5:1842:G:P      | 2.44                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 59:HH:93:VAL:HG21 | 59:HH:133:LEU:HD23 | 1.84                     | 0.57              |
| 48:5:1757:U:H2'   | 48:5:1758:G:O4'    | 2.03                     | 0.57              |
| 19:T:80:VAL:HG21  | 19:T:85:LEU:HD12   | 1.86                     | 0.57              |
| 1:A:207:VAL:HG11  | 48:5:1633:G:C6     | 2.38                     | 0.57              |
| 11:L:42:ARG:HG3   | 11:L:45:ARG:HH12   | 1.69                     | 0.57              |
| 51:9:1233:G:C2'   | 51:9:1234:C:H5'    | 2.34                     | 0.57              |
| 11:L:71:ARG:NH2   | 48:5:74:G:O3'      | 2.36                     | 0.57              |
| 74:WW:30:CYS:SG   | 74:WW:31:SER:N     | 2.77                     | 0.57              |
| 50:8:83:C:H4'     | 50:8:85:U:O2       | 2.03                     | 0.57              |
| 48:5:3751:G:O2'   | 48:5:3775:A:N6     | 2.37                     | 0.57              |
| 51:9:1406:G:H2'   | 51:9:1407:U:O3'    | 2.04                     | 0.57              |
| 6:F:91:LEU:HD22   | 6:F:92:ALA:N       | 2.20                     | 0.57              |
| 48:5:4461:C:O2    | 48:5:4516:G:C2     | 2.58                     | 0.57              |
| 48:5:2256:C:H2'   | 48:5:2256:C:O2     | 2.04                     | 0.57              |
| 1:A:101:VAL:HB    | 1:A:165:VAL:HG12   | 1.86                     | 0.57              |
| 48:5:4975:G:N2    | 48:5:4984:C:C2     | 2.72                     | 0.57              |
| 48:5:2367:A:N6    | 48:5:2798:A:O4'    | 2.37                     | 0.57              |
| 51:9:1212:G:O2'   | 51:9:1213:C:O4'    | 2.22                     | 0.57              |
| 51:9:1233:G:C6    | 51:9:1234:C:C4     | 2.93                     | 0.57              |
| 48:5:1639:U:N3    | 48:5:1643:A:O2'    | 2.37                     | 0.57              |
| 14:O:7:LEU:HD22   | 14:O:9:LEU:HD21    | 1.86                     | 0.57              |
| 4:D:62:CYS:HB3    | 4:D:105:LEU:HD22   | 1.87                     | 0.57              |
| 51:9:316:G:N1     | 51:9:317:C:C4      | 2.72                     | 0.57              |
| 48:5:1279:A:OP1   | 48:5:1279:A:O3'    | 2.22                     | 0.57              |
| 48:5:3870:C:C2    | 48:5:3886:G:C2     | 2.92                     | 0.57              |
| 51:9:1347:U:H2'   | 51:9:1348:G:C8     | 2.39                     | 0.57              |
| 51:9:322:C:O2'    | 51:9:323:C:OP2     | 2.21                     | 0.57              |
| 48:5:2408:U:C1'   | 48:5:2409:U:C5     | 2.88                     | 0.57              |
| 50:8:55:U:C4      | 50:8:62:A:N1       | 2.72                     | 0.57              |
| 3:C:313:VAL:CG1   | 6:F:172:THR:HG21   | 2.35                     | 0.57              |
| 51:9:195:C:C2     | 51:9:205:G:N2      | 2.73                     | 0.57              |
| 47:3:35:U:O4'     | 51:9:1641:A:OP1    | 2.22                     | 0.56              |
| 48:5:2773:G:N1    | 48:5:2774:C:C4     | 2.73                     | 0.56              |
| 76:YY:113:ARG:O   | 76:YY:114:MET:HB2  | 2.05                     | 0.56              |
| 48:5:685:C:O2     | 48:5:685:C:C2'     | 2.53                     | 0.56              |
| 3:C:336:ARG:O     | 3:C:340:ILE:HG12   | 2.05                     | 0.56              |
| 53:BB:141:GLY:HA2 | 53:BB:210:VAL:HG22 | 1.87                     | 0.56              |
| 61:JJ:125:HIS:NE2 | 61:JJ:129:LEU:HD21 | 2.20                     | 0.56              |
| 48:5:1365:C:H4'   | 48:5:1366:G:OP1    | 2.05                     | 0.56              |
| 51:9:1137:U:H3    | 51:9:1148:A:N6     | 2.03                     | 0.56              |
| 7:G:156:VAL:CG1   | 7:G:184:LEU:CD1    | 2.78                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 48:5:2409:U:C5   | 48:5:2783:A:C2    | 2.93                     | 0.56              |
| 51:9:1760:G:C2   | 51:9:1773:C:C2    | 2.93                     | 0.56              |
| 7:G:86:VAL:HG22  | 7:G:183:ILE:HG22  | 1.87                     | 0.56              |
| 51:9:911:C:O2'   | 51:9:912:C:H5'    | 2.05                     | 0.56              |
| 10:J:83:LEU:CD1  | 10:J:170:TYR:CZ   | 2.87                     | 0.56              |
| 48:5:516:C:N3    | 48:5:646:G:C2     | 2.74                     | 0.56              |
| 23:X:139:ARG:NH2 | 48:5:2533:C:OP1   | 2.38                     | 0.56              |
| 48:5:665:C:H2'   | 48:5:665:C:O2     | 2.05                     | 0.56              |
| 49:7:66:G:C2     | 49:7:67:C:C2      | 2.93                     | 0.56              |
| 48:5:3709:U:O2'  | 48:5:3710:G:O4'   | 2.21                     | 0.56              |
| 58:GG:214:ALA:O  | 58:GG:218:LYS:N   | 2.36                     | 0.56              |
| 48:5:1278:C:C6   | 48:5:1279:A:H1'   | 2.40                     | 0.56              |
| 51:9:830:A:N1    | 51:9:844:U:C4     | 2.74                     | 0.56              |
| 47:3:39:U:O2'    | 47:3:40:C:C6      | 2.57                     | 0.56              |
| 48:5:1398:A:O2'  | 48:5:1399:G:OP2   | 2.20                     | 0.56              |
| 51:9:167:G:C6    | 51:9:168:C:C5     | 2.94                     | 0.56              |
| 19:T:64:VAL:HG13 | 19:T:72:VAL:HG13  | 1.88                     | 0.56              |
| 51:9:1009:A:O2'  | 65:NN:114:ARG:HG3 | 2.05                     | 0.56              |
| 48:5:2258:C:C2'  | 48:5:2258:C:O2    | 2.54                     | 0.56              |
| 48:5:2640:G:N7   | 48:5:2694:G:O6    | 2.37                     | 0.56              |
| 48:5:2524:U:H5'' | 48:5:2711:G:C2    | 2.40                     | 0.56              |
| 48:5:4101:C:C2   | 48:5:4109:G:C2    | 2.94                     | 0.56              |
| 48:5:746:A:O2'   | 48:5:747:A:O5'    | 2.20                     | 0.56              |
| 48:5:1268:G:C4   | 48:5:2111:G:C2    | 2.93                     | 0.56              |
| 48:5:1666:C:O2'  | 48:5:1688:G:OP1   | 2.21                     | 0.56              |
| 51:9:1545:A:H2'  | 51:9:1546:G:C8    | 2.41                     | 0.56              |
| 48:5:3759:A:N1   | 51:9:1708:C:O2'   | 2.30                     | 0.56              |
| 17:R:60:ARG:NH1  | 17:R:63:CYS:SG    | 2.79                     | 0.56              |
| 48:5:4260:U:H2'  | 48:5:4261:C:C6    | 2.40                     | 0.56              |
| 49:7:30:C:C2     | 49:7:48:G:C2      | 2.94                     | 0.56              |
| 53:BB:85:LYS:HB3 | 53:BB:101:HIS:HB3 | 1.88                     | 0.56              |
| 6:F:146:TYR:CE2  | 6:F:239:GLU:HB3   | 2.41                     | 0.56              |
| 48:5:976:G:C6    | 48:5:977:C:C4     | 2.93                     | 0.56              |
| 48:5:1279:A:H2'  | 48:5:1280:C:H5''  | 1.88                     | 0.56              |
| 48:5:1360:G:C6   | 48:5:1361:G:C5    | 2.94                     | 0.56              |
| 51:9:1231:C:H2'  | 51:9:1232:U:O4'   | 2.05                     | 0.56              |
| 51:9:434:G:H2'   | 51:9:435:A:C8     | 2.41                     | 0.56              |
| 51:9:1643:U:H2'  | 51:9:1644:C:C6    | 2.40                     | 0.56              |
| 48:5:4416:G:N2   | 48:5:4417:C:C2    | 2.74                     | 0.56              |
| 3:C:114:ARG:CZ   | 48:5:1358:G:H5''  | 2.36                     | 0.56              |
| 48:5:1404:G:N2   | 48:5:1414:C:C2    | 2.74                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:2555:G:O6    | 48:5:2572:C:N4    | 2.37                     | 0.56              |
| 50:8:155:C:H2'    | 50:8:156:U:O4'    | 2.05                     | 0.56              |
| 51:9:1613:G:C2    | 51:9:1627:C:C2    | 2.93                     | 0.56              |
| 59:HH:39:GLN:HG3  | 59:HH:75:ILE:HD12 | 1.87                     | 0.56              |
| 49:7:82:G:C2      | 49:7:95:C:C2      | 2.94                     | 0.56              |
| 48:5:370:U:C6     | 48:5:1637:A:C2    | 2.93                     | 0.56              |
| 48:5:1959:U:H1'   | 48:5:1961:G:N9    | 2.21                     | 0.56              |
| 48:5:2028:C:O2'   | 48:5:2029:A:O5'   | 2.24                     | 0.56              |
| 48:5:3593:C:H4'   | 48:5:3594:C:OP2   | 2.05                     | 0.56              |
| 48:5:466:A:C2     | 48:5:467:U:C4     | 2.94                     | 0.56              |
| 47:3:41:U:H4'     | 57:FF:198:ARG:HD3 | 1.88                     | 0.55              |
| 48:5:1269:G:C6    | 48:5:2111:G:N2    | 2.74                     | 0.55              |
| 48:5:2481:G:C2    | 48:5:2498:C:C2    | 2.94                     | 0.55              |
| 51:9:1500:G:C6    | 51:9:1501:C:C4    | 2.94                     | 0.55              |
| 51:9:1520:G:N3    | 51:9:1520:G:H2'   | 2.20                     | 0.55              |
| 51:9:1117:C:O2    | 51:9:1117:C:O4'   | 2.25                     | 0.55              |
| 15:P:36:ILE:HD12  | 15:P:48:LEU:HD11  | 1.88                     | 0.55              |
| 48:5:2256:C:O2    | 48:5:2256:C:C2'   | 2.54                     | 0.55              |
| 14:O:18:ARG:NH1   | 48:5:2053:C:O3'   | 2.38                     | 0.55              |
| 17:R:10:LEU:HB3   | 17:R:41:ILE:HD13  | 1.88                     | 0.55              |
| 48:5:1277:G:N2    | 48:5:1278:C:C2    | 2.75                     | 0.55              |
| 47:3:39:U:O2'     | 47:3:40:C:C5'     | 2.54                     | 0.55              |
| 48:5:2547:G:N1    | 48:5:2548:C:C4    | 2.75                     | 0.55              |
| 48:5:4586:G:H5''  | 48:5:4586:G:H8    | 1.70                     | 0.55              |
| 54:CC:75:ILE:HG23 | 54:CC:80:GLU:OE1  | 2.06                     | 0.55              |
| 48:5:106:A:H2'    | 48:5:107:G:O4'    | 2.06                     | 0.55              |
| 47:3:37:A:H2'     | 47:3:38:A:H5'     | 1.88                     | 0.55              |
| 48:5:3612:C:H1'   | 48:5:5016:A:C8    | 2.41                     | 0.55              |
| 48:5:2557:G:C2    | 48:5:2571:C:C2    | 2.94                     | 0.55              |
| 51:9:642:U:H4'    | 51:9:643:A:OP1    | 2.05                     | 0.55              |
| 48:5:181:C:N4     | 48:5:256:G:C6     | 2.74                     | 0.55              |
| 48:5:497:G:C2     | 48:5:657:C:C2     | 2.94                     | 0.55              |
| 15:P:48:LEU:HD12  | 15:P:92:LEU:HD13  | 1.87                     | 0.55              |
| 15:P:69:ARG:NH2   | 48:5:4568:A:N3    | 2.55                     | 0.55              |
| 48:5:2408:U:O4'   | 48:5:2409:U:C5    | 2.60                     | 0.55              |
| 3:C:158:VAL:HG22  | 3:C:161:TYR:HE2   | 1.71                     | 0.55              |
| 51:9:145:G:N7     | 58:GG:178:ARG:NH1 | 2.54                     | 0.55              |
| 48:5:937:U:H2'    | 48:5:937:U:O2     | 2.07                     | 0.55              |
| 51:9:1282:A:H3'   | 51:9:1283:C:C5'   | 2.36                     | 0.55              |
| 48:5:4524:G:N2    | 48:5:4525:C:C2    | 2.75                     | 0.55              |
| 48:5:1279:A:C2    | 48:5:1280:C:C2    | 2.95                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:1743:A:C5    | 48:5:1744:U:C5     | 2.95                     | 0.55              |
| 65:NN:54:LEU:HB3  | 65:NN:60:VAL:HG13  | 1.88                     | 0.55              |
| 48:5:1751:A:C2    | 48:5:1780:A:C2     | 2.95                     | 0.55              |
| 45:1:68:VAL:C     | 46:2:76:A:O2'      | 2.45                     | 0.55              |
| 48:5:1371:A:N6    | 50:8:28:C:O2'      | 2.40                     | 0.55              |
| 51:9:1741:U:H2'   | 51:9:1742:C:O4'    | 2.06                     | 0.55              |
| 51:9:1408:U:C4    | 51:9:1409:A:N6     | 2.74                     | 0.55              |
| 48:5:919:C:N4     | 48:5:920:C:C5      | 2.75                     | 0.55              |
| 56:EE:55:ALA:HB1  | 56:EE:60:GLU:HB2   | 1.88                     | 0.55              |
| 48:5:933:G:C2     | 48:5:940:C:C6      | 2.95                     | 0.55              |
| 51:9:1698:C:O2    | 51:9:1698:C:O4'    | 2.23                     | 0.55              |
| 48:5:3641:U:H5    | 48:5:3646:A:N7     | 2.04                     | 0.55              |
| 48:5:422:C:C2     | 50:8:13:G:C2       | 2.94                     | 0.55              |
| 51:9:115:U:H2'    | 51:9:116:U:C6      | 2.41                     | 0.55              |
| 51:9:1137:U:HO2'  | 52:AA:155:ARG:HH22 | 1.55                     | 0.55              |
| 5:E:238:ILE:C     | 5:E:239:THR:HG1    | 1.99                     | 0.55              |
| 51:9:1102:G:N2    | 51:9:1130:G:N2     | 2.55                     | 0.55              |
| 51:9:1616:U:O4    | 67:PP:40:ARG:NH1   | 2.40                     | 0.55              |
| 3:C:168:VAL:HG13  | 3:C:177:TRP:CZ3    | 2.41                     | 0.55              |
| 48:5:962:C:OP2    | 48:5:2264:C:N3     | 2.40                     | 0.55              |
| 48:5:1975:G:O4'   | 48:5:1984:A:H1'    | 2.07                     | 0.55              |
| 47:3:76:A:C5      | 48:5:4371:G:C5     | 2.94                     | 0.55              |
| 51:9:1526:G:N1    | 51:9:1527:C:C4     | 2.75                     | 0.55              |
| 48:5:2089:G:O2'   | 48:5:2090:U:OP2    | 2.25                     | 0.55              |
| 56:EE:64:ILE:HG23 | 76:YY:17:LEU:HD13  | 1.89                     | 0.55              |
| 17:R:71:ARG:NH1   | 48:5:3605:C:OP2    | 2.36                     | 0.55              |
| 48:5:1483:C:O4'   | 48:5:1483:C:O2     | 2.23                     | 0.55              |
| 48:5:1485:C:O4'   | 48:5:1485:C:O2     | 2.23                     | 0.55              |
| 48:5:127:G:N2     | 48:5:128:C:C2      | 2.75                     | 0.55              |
| 62:KK:11:ILE:HD12 | 62:KK:45:VAL:HG22  | 1.89                     | 0.55              |
| 51:9:698:G:N1     | 51:9:733:C:C2      | 2.75                     | 0.55              |
| 48:5:1249:C:C2    | 48:5:1262:G:C2     | 2.95                     | 0.55              |
| 48:5:3816:A:O2'   | 48:5:3819:G:N3     | 2.39                     | 0.55              |
| 51:9:832:G:C2     | 51:9:843:C:C2      | 2.95                     | 0.54              |
| 51:9:1760:G:N2    | 51:9:1773:C:C2     | 2.76                     | 0.54              |
| 48:5:2688:G:N2    | 48:5:2689:C:C2     | 2.75                     | 0.54              |
| 51:9:1265:A:H2'   | 51:9:1265:A:N3     | 2.21                     | 0.54              |
| 52:AA:42:LYS:CG   | 52:AA:48:ILE:HD11  | 2.36                     | 0.54              |
| 51:9:164:A:C2     | 51:9:165:G:C8      | 2.95                     | 0.54              |
| 48:5:1205:G:N2    | 48:5:1206:C:C2     | 2.76                     | 0.54              |
| 1:A:82:ILE:HD11   | 1:A:99:GLY:HA3     | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:9:1568:C:O2'   | 51:9:1569:A:O4'   | 2.24                     | 0.54              |
| 46:2:34:A:O2'     | 46:2:35:A:O4'     | 2.25                     | 0.54              |
| 72:UU:60:THR:HG22 | 72:UU:83:ARG:HG2  | 1.89                     | 0.54              |
| 6:F:230:VAL:HA    | 18:S:39:VAL:HG12  | 1.89                     | 0.54              |
| 48:5:4389:C:H2'   | 48:5:4390:A:C8    | 2.43                     | 0.54              |
| 48:5:1968:G:O2'   | 48:5:1969:G:O5'   | 2.20                     | 0.54              |
| 9:I:184:MET:HE2   | 9:I:190:LEU:CD1   | 2.36                     | 0.54              |
| 14:O:36:VAL:HG11  | 14:O:108:ILE:HD12 | 1.89                     | 0.54              |
| 19:T:87:LYS:NZ    | 48:5:4301:U:OP2   | 2.39                     | 0.54              |
| 48:5:3751:G:O2'   | 48:5:3752:C:C5'   | 2.47                     | 0.54              |
| 48:5:1563:A:C8    | 48:5:1563:A:O5'   | 2.60                     | 0.54              |
| 51:9:1384:C:H2'   | 51:9:1385:G:H5'   | 1.89                     | 0.54              |
| 51:9:1839:U:H2'   | 51:9:1840:U:O4'   | 2.08                     | 0.54              |
| 48:5:2905:C:C2    | 48:5:3590:G:C2    | 2.96                     | 0.54              |
| 48:5:2490:U:O2'   | 48:5:2491:C:O4'   | 2.23                     | 0.54              |
| 51:9:1220:A:N6    | 51:9:1221:G:C6    | 2.75                     | 0.54              |
| 48:5:1664:U:H2'   | 48:5:1665:C:C6    | 2.42                     | 0.54              |
| 2:B:163:LEU:HD23  | 2:B:182:GLU:HA    | 1.89                     | 0.54              |
| 51:9:1598:G:H3'   | 77:ZZ:80:ARG:HD2  | 1.89                     | 0.54              |
| 75:XX:68:LYS:HB3  | 75:XX:91:LEU:HD22 | 1.88                     | 0.54              |
| 47:3:16:C:O2      | 47:3:16:C:O4'     | 2.25                     | 0.54              |
| 48:5:5023:C:O2    | 48:5:5023:C:O4'   | 2.23                     | 0.54              |
| 53:BB:88:THR:HG22 | 53:BB:96:CYS:HB3  | 1.88                     | 0.54              |
| 56:EE:195:ILE:O   | 56:EE:196:THR:CB  | 2.55                     | 0.54              |
| 11:L:47:ALA:HB3   | 11:L:48:PRO:HD3   | 1.87                     | 0.54              |
| 48:5:4213:A:H61   | 48:5:4218:U:H3    | 1.55                     | 0.54              |
| 51:9:1144:A:C2    | 51:9:1145:A:C2    | 2.95                     | 0.54              |
| 51:9:1129:G:H3'   | 51:9:1130:G:H8    | 1.72                     | 0.54              |
| 48:5:516:C:C2     | 48:5:646:G:C2     | 2.95                     | 0.54              |
| 47:3:38:A:C2      | 57:FF:135:ARG:NH1 | 2.75                     | 0.54              |
| 48:5:2089:G:N3    | 48:5:2089:G:H2'   | 2.23                     | 0.54              |
| 48:5:4730:C:O4'   | 48:5:4730:C:O2    | 2.24                     | 0.54              |
| 65:NN:40:LEU:HD22 | 65:NN:45:LEU:HD12 | 1.90                     | 0.54              |
| 51:9:1403:C:O2    | 51:9:1403:C:C2'   | 2.54                     | 0.54              |
| 3:C:114:ARG:NE    | 48:5:1358:G:O3'   | 2.37                     | 0.54              |
| 48:5:1067:G:H2'   | 48:5:1068:G:O4'   | 2.07                     | 0.54              |
| 48:5:3662:A:N6    | 48:5:3680:U:H3    | 2.06                     | 0.54              |
| 51:9:1241:A:C2    | 51:9:1517:G:O4'   | 2.61                     | 0.54              |
| 16:Q:69:LYS:O     | 16:Q:75:ARG:NH1   | 2.39                     | 0.54              |
| 48:5:2367:A:C2    | 48:5:2788:U:O4    | 2.53                     | 0.54              |
| 48:5:1380:G:H4'   | 48:5:1381:U:OP1   | 2.07                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:3:76:A:N7       | 48:5:4371:G:N1    | 2.56                     | 0.54              |
| 48:5:5061:A:O2'    | 48:5:5062:G:OP2   | 2.11                     | 0.54              |
| 13:N:135:ILE:HD12  | 13:N:151:ILE:HD13 | 1.90                     | 0.54              |
| 48:5:4895:C:H1'    | 48:5:4896:G:C8    | 2.43                     | 0.54              |
| 48:5:1959:U:H4'    | 48:5:1961:G:C4'   | 2.37                     | 0.54              |
| 47:3:76:A:C8       | 48:5:4341:C:N4    | 2.74                     | 0.54              |
| 49:7:66:G:C6       | 49:7:67:C:C4      | 2.95                     | 0.54              |
| 1:A:196:TRP:O      | 1:A:197:PRO:C     | 2.46                     | 0.54              |
| 2:B:116:ARG:HD2    | 2:B:122:TRP:CD2   | 2.43                     | 0.54              |
| 51:9:1374:C:H2'    | 51:9:1375:G:O4'   | 2.08                     | 0.54              |
| 67:PP:17:TYR:OH    | 67:PP:37:TYR:HB3  | 2.08                     | 0.54              |
| 51:9:669:A:N3      | 51:9:1164:G:O2'   | 2.38                     | 0.54              |
| 48:5:301:G:C6      | 48:5:302:C:C4     | 2.96                     | 0.53              |
| 53:BB:119:THR:H    | 53:BB:143:THR:HG1 | 1.54                     | 0.53              |
| 74:WW:52:ILE:HG22  | 74:WW:61:ILE:HG12 | 1.89                     | 0.53              |
| 48:5:1468:C:C2     | 48:5:1498:G:C2    | 2.96                     | 0.53              |
| 48:5:1357:C:H5''   | 48:5:1358:G:OP1   | 2.08                     | 0.53              |
| 47:3:76:A:N6       | 48:5:4371:G:C5    | 2.77                     | 0.53              |
| 51:9:522:A:O2'     | 61:JJ:131:ARG:NH2 | 2.42                     | 0.53              |
| 51:9:522:A:OP2     | 61:JJ:45:ARG:NH2  | 2.42                     | 0.53              |
| 48:5:3718:A:H2'    | 48:5:3719:A:C8    | 2.43                     | 0.53              |
| 51:9:750:C:H2'     | 51:9:750:C:O2     | 2.08                     | 0.53              |
| 48:5:4717:A:H2'    | 48:5:4718:G:O4'   | 2.07                     | 0.53              |
| 19:T:48:VAL:HG21   | 19:T:94:GLU:HG2   | 1.90                     | 0.53              |
| 48:5:1358:G:O2'    | 48:5:1359:G:O4'   | 2.20                     | 0.53              |
| 56:EE:126:VAL:HG22 | 56:EE:158:ASP:O   | 2.08                     | 0.53              |
| 51:9:71:G:O2'      | 51:9:72:C:OP1     | 2.20                     | 0.53              |
| 48:5:2301:G:N2     | 48:5:2302:C:C2    | 2.76                     | 0.53              |
| 48:5:1668:A:C4     | 48:5:2282:A:C2    | 2.96                     | 0.53              |
| 48:5:1430:C:C2     | 48:5:1455:G:C2    | 2.96                     | 0.53              |
| 47:3:34:U:O2       | 51:9:1641:A:OP1   | 2.26                     | 0.53              |
| 48:5:3914:U:N3     | 48:5:4378:A:N6    | 2.48                     | 0.53              |
| 51:9:1543:U:OP2    | 71:TT:62:ARG:NH1  | 2.41                     | 0.53              |
| 51:9:1348:G:H1     | 51:9:1381:G:H22   | 1.57                     | 0.53              |
| 51:9:823:U:O4'     | 51:9:823:U:O2     | 2.25                     | 0.53              |
| 51:9:216:C:O4'     | 51:9:216:C:O2     | 2.24                     | 0.53              |
| 48:5:4635:A:C2     | 48:5:4664:A:C5    | 2.96                     | 0.53              |
| 10:J:119:TYR:HB3   | 70:SS:12:ILE:HD13 | 1.89                     | 0.53              |
| 48:5:4723:A:C2     | 48:5:4724:A:C5    | 2.97                     | 0.53              |
| 48:5:4583:C:C4     | 48:5:4718:G:C6    | 2.96                     | 0.53              |
| 51:9:686:U:O2      | 59:HH:118:ARG:NH2 | 2.32                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:5:1086:C:C2     | 48:5:1212:G:C2    | 2.97                     | 0.53              |
| 51:9:501:C:H2'     | 51:9:501:C:O2     | 2.08                     | 0.53              |
| 5:E:126:ARG:HH12   | 48:5:712:C:H2'    | 1.69                     | 0.53              |
| 5:E:202:VAL:HB     | 5:E:252:GLN:OE1   | 2.09                     | 0.53              |
| 51:9:1386:A:H2'    | 51:9:1387:G:C8    | 2.43                     | 0.53              |
| 48:5:2108:G:N1     | 48:5:2125:C:C4    | 2.77                     | 0.53              |
| 48:5:1297:U:O4'    | 48:5:1297:U:OP2   | 2.27                     | 0.53              |
| 6:F:244:ARG:NH1    | 48:5:942:G:OP2    | 2.42                     | 0.53              |
| 53:BB:143:THR:HG22 | 53:BB:205:TYR:CD1 | 2.43                     | 0.53              |
| 50:8:15:G:C6       | 50:8:16:G:N1      | 2.76                     | 0.53              |
| 48:5:4977:A:H2'    | 48:5:4978:G:O4'   | 2.08                     | 0.53              |
| 48:5:5026:U:H5'    | 60:II:79:ILE:HD11 | 1.90                     | 0.53              |
| 48:5:199:G:C2      | 48:5:220:C:O2     | 2.62                     | 0.53              |
| 56:EE:31:PRO:HD3   | 56:EE:38:LEU:HD13 | 1.90                     | 0.53              |
| 3:C:130:ALA:HB1    | 3:C:136:LEU:HD12  | 1.91                     | 0.53              |
| 48:5:1398:A:H1'    | 48:5:1399:G:C8    | 2.43                     | 0.53              |
| 7:G:156:VAL:HG13   | 7:G:184:LEU:HG    | 1.89                     | 0.53              |
| 51:9:167:G:N1      | 51:9:168:C:C4     | 2.77                     | 0.53              |
| 48:5:2693:G:C6     | 48:5:2694:G:N1    | 2.77                     | 0.53              |
| 51:9:71:G:H3'      | 51:9:72:C:H5''    | 1.91                     | 0.53              |
| 48:5:1213:G:C6     | 48:5:1215:C:N3    | 2.77                     | 0.53              |
| 48:5:986:C:C2      | 48:5:1068:G:C2    | 2.97                     | 0.53              |
| 51:9:1599:U:O2     | 51:9:1599:U:O4'   | 2.24                     | 0.53              |
| 48:5:1447:C:H2'    | 48:5:1448:G:O4'   | 2.08                     | 0.53              |
| 17:R:95:TRP:CH2    | 17:R:99:MET:HE2   | 2.44                     | 0.53              |
| 46:2:39:G:N2       | 46:2:40:C:C2      | 2.76                     | 0.53              |
| 48:5:2654:C:C2     | 48:5:2681:G:C2    | 2.97                     | 0.53              |
| 14:O:72:HIS:N      | 48:5:4586:G:OP1   | 2.39                     | 0.53              |
| 48:5:5028:G:C6     | 48:5:5029:C:N4    | 2.77                     | 0.53              |
| 69:RR:16:ILE:HG22  | 69:RR:24:LEU:HD11 | 1.91                     | 0.53              |
| 51:9:55:U:C2'      | 51:9:55:U:O2      | 2.56                     | 0.53              |
| 10:J:53:ALA:HB2    | 10:J:68:ILE:HD12  | 1.91                     | 0.53              |
| 48:5:677:G:N2      | 48:5:678:C:C2     | 2.77                     | 0.53              |
| 7:G:29:ASN:HB2     | 7:G:32:PHE:CE2    | 2.43                     | 0.53              |
| 51:9:944:A:C5      | 51:9:945:U:C5     | 2.97                     | 0.52              |
| 48:5:256:G:N2      | 48:5:257:C:C2     | 2.77                     | 0.52              |
| 48:5:3594:C:O2     | 48:5:3594:C:C2'   | 2.56                     | 0.52              |
| 8:H:26:ILE:HB      | 8:H:35:ARG:HG2    | 1.91                     | 0.52              |
| 48:5:1822:U:O2     | 48:5:1822:U:O4'   | 2.27                     | 0.52              |
| 25:Z:29:ILE:HG21   | 25:Z:40:HIS:CE1   | 2.44                     | 0.52              |
| 11:L:9:ILE:O       | 11:L:9:ILE:HG23   | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:977:C:N3      | 48:5:978:G:N7      | 2.57                     | 0.52              |
| 48:5:4579:U:H2'    | 48:5:4580:U:O4'    | 2.08                     | 0.52              |
| 51:9:834:C:C2      | 51:9:841:G:N2      | 2.78                     | 0.52              |
| 48:5:707:C:O2      | 48:5:1291:G:C2     | 2.63                     | 0.52              |
| 48:5:2043:A:O2'    | 48:5:4461:C:O2     | 2.25                     | 0.52              |
| 48:5:4759:C:H2'    | 48:5:4760:G:O4'    | 2.09                     | 0.52              |
| 17:R:35:ALA:O      | 17:R:37:SER:N      | 2.41                     | 0.52              |
| 48:5:4883:C:HO2'   | 48:5:4884:G:P      | 2.32                     | 0.52              |
| 66:OO:56:VAL:HG12  | 66:OO:81:VAL:HG23  | 1.92                     | 0.52              |
| 48:5:4281:A:C2     | 48:5:4283:G:C5     | 2.98                     | 0.52              |
| 51:9:50:A:C2       | 51:9:488:U:O4      | 2.63                     | 0.52              |
| 48:5:2108:G:C2     | 48:5:2125:C:N3     | 2.77                     | 0.52              |
| 51:9:409:C:C2      | 51:9:432:G:C2      | 2.97                     | 0.52              |
| 51:9:1553:C:O2     | 51:9:1553:C:O4'    | 2.25                     | 0.52              |
| 48:5:2110:C:C6     | 48:5:2110:C:OP1    | 2.62                     | 0.52              |
| 48:5:4138:C:C2     | 48:5:4147:G:C2     | 2.96                     | 0.52              |
| 48:5:1899:G:N2     | 48:5:1900:C:C2     | 2.77                     | 0.52              |
| 11:L:58:ILE:HG23   | 11:L:70:VAL:CG1    | 2.39                     | 0.52              |
| 51:9:873:G:N1      | 51:9:914:U:C5      | 2.77                     | 0.52              |
| 48:5:4441:A:C8     | 48:5:4441:A:H5''   | 2.44                     | 0.52              |
| 63:LL:113:LEU:HD23 | 63:LL:142:VAL:HG21 | 1.90                     | 0.52              |
| 48:5:43:U:H2'      | 48:5:44:A:O5'      | 2.09                     | 0.52              |
| 17:R:59:SER:N      | 48:5:4646:U:OP1    | 2.42                     | 0.52              |
| 48:5:112:C:C2      | 48:5:330:G:C2      | 2.97                     | 0.52              |
| 47:3:6:G:N2        | 47:3:67:U:O2       | 2.42                     | 0.52              |
| 48:5:1378:C:OP1    | 48:5:1379:C:H3'    | 2.09                     | 0.52              |
| 48:5:181:C:C2      | 48:5:256:G:C2      | 2.98                     | 0.52              |
| 51:9:1265:A:C2'    | 51:9:1265:A:N3     | 2.73                     | 0.52              |
| 52:AA:123:VAL:HG13 | 52:AA:145:ILE:HB   | 1.92                     | 0.52              |
| 48:5:12:A:H8       | 48:5:12:A:H5''     | 1.75                     | 0.52              |
| 51:9:853:C:O4'     | 51:9:853:C:O2      | 2.28                     | 0.52              |
| 70:SS:27:ALA:HB1   | 70:SS:42:HIS:CE1   | 2.43                     | 0.52              |
| 48:5:2733:C:H2'    | 48:5:2734:U:O4'    | 2.10                     | 0.52              |
| 54:CC:165:VAL:HG21 | 54:CC:217:ALA:HB1  | 1.91                     | 0.52              |
| 48:5:2638:G:C2     | 48:5:2639:U:C4     | 2.98                     | 0.52              |
| 56:EE:129:ILE:HD13 | 56:EE:155:LYS:HA   | 1.90                     | 0.52              |
| 48:5:300:A:H2'     | 48:5:301:G:C8      | 2.45                     | 0.52              |
| 51:9:350:C:HO2'    | 51:9:383:G:N2      | 2.06                     | 0.52              |
| 4:D:129:GLU:HG3    | 4:D:177:THR:HG21   | 1.90                     | 0.52              |
| 48:5:1874:A:H5'    | 48:5:4218:U:O2     | 2.10                     | 0.52              |
| 48:5:4338:G:C4     | 48:5:4372:U:C5     | 2.98                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1912:G:N2     | 48:5:1913:C:C2     | 2.78                     | 0.52              |
| 48:5:1854:G:N2     | 48:5:4394:A:O4'    | 2.42                     | 0.52              |
| 51:9:1696:C:HO2'   | 51:9:1702:G:HO2'   | 1.57                     | 0.52              |
| 48:5:52:G:N2       | 48:5:53:C:C2       | 2.78                     | 0.52              |
| 59:HH:43:LEU:HD21  | 59:HH:71:SER:HB3   | 1.92                     | 0.52              |
| 5:E:62:LYS:HE2     | 48:5:979:C:OP2     | 2.10                     | 0.52              |
| 17:R:95:TRP:CZ2    | 17:R:99:MET:HE2    | 2.45                     | 0.52              |
| 51:9:751:G:C6      | 51:9:792:C:N4      | 2.78                     | 0.52              |
| 48:5:1266:G:H5''   | 48:5:2112:G:N3     | 2.25                     | 0.52              |
| 51:9:834:C:H3'     | 51:9:835:C:H4'     | 1.91                     | 0.52              |
| 56:EE:49:ARG:HB3   | 56:EE:55:ALA:HB3   | 1.92                     | 0.52              |
| 2:B:29:VAL:HG13    | 2:B:348:ARG:HD3    | 1.91                     | 0.52              |
| 57:FF:102:LEU:HD11 | 77:ZZ:100:VAL:HG21 | 1.92                     | 0.52              |
| 51:9:49:C:O2       | 51:9:478:G:C2      | 2.63                     | 0.52              |
| 51:9:1407:U:C2'    | 51:9:1408:U:C6     | 2.91                     | 0.52              |
| 51:9:1386:A:OP1    | 51:9:1483:A:N3     | 2.43                     | 0.52              |
| 51:9:980:A:C2      | 51:9:981:A:C6      | 2.98                     | 0.52              |
| 2:B:154:LYS:HB2    | 2:B:154:LYS:HZ2    | 1.75                     | 0.52              |
| 51:9:312:G:O2'     | 51:9:313:A:OP1     | 2.19                     | 0.52              |
| 48:5:4735:G:C2     | 48:5:4736:C:C2     | 2.98                     | 0.52              |
| 51:9:507:G:OP1     | 76:YY:108:LYS:NZ   | 2.40                     | 0.52              |
| 48:5:211:G:H4'     | 48:5:234:G:C8      | 2.45                     | 0.52              |
| 51:9:437:G:C2      | 51:9:457:C:C2      | 2.98                     | 0.52              |
| 56:EE:11:ARG:HD2   | 56:EE:20:LEU:HB3   | 1.90                     | 0.52              |
| 48:5:1549:G:C2     | 48:5:1580:C:C2     | 2.98                     | 0.52              |
| 51:9:1235:G:C5'    | 51:9:1247:C:H42    | 2.13                     | 0.51              |
| 47:3:76:A:C5       | 48:5:4371:G:C6     | 2.98                     | 0.51              |
| 48:5:2525:U:P      | 48:5:2711:G:H1     | 2.33                     | 0.51              |
| 48:5:915:A:HO2'    | 48:5:916:C:H6      | 1.58                     | 0.51              |
| 51:9:963:A:H2'     | 51:9:964:A:O4'     | 2.09                     | 0.51              |
| 63:LL:61:PRO:HA    | 63:LL:66:VAL:HG13  | 1.92                     | 0.51              |
| 4:D:196:ARG:O      | 4:D:200:MET:HG2    | 2.10                     | 0.51              |
| 48:5:1771:U:H2'    | 48:5:1772:C:O4'    | 2.10                     | 0.51              |
| 51:9:398:A:H5'     | 51:9:398:A:C8      | 2.46                     | 0.51              |
| 51:9:1118:C:O2     | 51:9:1118:C:O4'    | 2.25                     | 0.51              |
| 48:5:1904:G:C2     | 48:5:2073:C:C2     | 2.98                     | 0.51              |
| 50:8:119:C:C2      | 50:8:132:G:C2      | 2.98                     | 0.51              |
| 5:E:250:ASP:O      | 5:E:254:LEU:HB2    | 2.10                     | 0.51              |
| 48:5:1358:G:H2'    | 48:5:1359:G:H8     | 1.75                     | 0.51              |
| 48:5:1268:G:C2     | 48:5:2111:G:N2     | 2.78                     | 0.51              |
| 25:Z:51:ARG:HB2    | 25:Z:65:ARG:HD2    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:5000:G:N2    | 48:5:5051:C:C2    | 2.78                     | 0.51              |
| 2:B:21:ARG:NH2    | 48:5:4568:A:O3'   | 2.44                     | 0.51              |
| 48:5:1736:A:N3    | 49:7:78:C:O2'     | 2.42                     | 0.51              |
| 48:5:4966:A:H2'   | 48:5:4967:A:C8    | 2.45                     | 0.51              |
| 9:I:187:GLU:OE1   | 9:I:189:ARG:CD    | 2.58                     | 0.51              |
| 54:CC:192:LEU:HB3 | 54:CC:227:TRP:HD1 | 1.74                     | 0.51              |
| 4:D:200:MET:HE1   | 4:D:241:LYS:CE    | 2.40                     | 0.51              |
| 48:5:5026:U:C6    | 60:II:79:ILE:HG13 | 2.45                     | 0.51              |
| 48:5:1723:A:N1    | 48:5:1838:A:N1    | 2.58                     | 0.51              |
| 51:9:1588:A:H2'   | 51:9:1589:A:C8    | 2.46                     | 0.51              |
| 51:9:195:C:C2     | 51:9:205:G:C2     | 2.99                     | 0.51              |
| 48:5:3641:U:C2    | 48:5:3645:U:C5    | 2.99                     | 0.51              |
| 48:5:470:A:C5     | 48:5:471:A:C8     | 2.99                     | 0.51              |
| 2:B:56:ILE:HG12   | 2:B:365:LEU:HD22  | 1.92                     | 0.51              |
| 46:2:16:C:O2      | 46:2:16:C:O4'     | 2.24                     | 0.51              |
| 48:5:2297:G:N2    | 48:5:2338:C:C2    | 2.79                     | 0.51              |
| 7:G:34:LYS:O      | 48:5:4128:A:N3    | 2.43                     | 0.51              |
| 48:5:1959:U:H4'   | 48:5:1961:G:C5'   | 2.41                     | 0.51              |
| 48:5:2301:G:N1    | 48:5:2302:C:C4    | 2.79                     | 0.51              |
| 51:9:599:A:H2'    | 51:9:606:G:N2     | 2.25                     | 0.51              |
| 48:5:2505:C:O2    | 48:5:2505:C:O4'   | 2.28                     | 0.51              |
| 4:D:122:GLN:O     | 4:D:248:ARG:NH2   | 2.43                     | 0.51              |
| 48:5:4305:G:C2'   | 48:5:4305:G:N3    | 2.73                     | 0.51              |
| 48:5:671:G:C6     | 48:5:672:C:C4     | 2.98                     | 0.51              |
| 58:GG:74:ARG:HA   | 58:GG:96:SER:HA   | 1.91                     | 0.51              |
| 48:5:2363:A:C2    | 48:5:3860:A:C4    | 2.98                     | 0.51              |
| 10:J:63:ARG:NH2   | 50:8:58:G:N7      | 129.21                   | 0.51              |
| 48:5:2026:A:H2'   | 48:5:2027:U:H5'   | 1.93                     | 0.51              |
| 51:9:305:U:H1'    | 60:II:55:TYR:CG   | 2.45                     | 0.51              |
| 51:9:1466:G:N1    | 51:9:1467:C:C4    | 2.79                     | 0.51              |
| 48:5:1891:A:O2'   | 48:5:1892:A:O4'   | 2.25                     | 0.51              |
| 51:9:412:G:C2     | 51:9:429:C:C2     | 2.99                     | 0.51              |
| 51:9:1500:G:C2    | 51:9:1501:C:C2    | 2.98                     | 0.51              |
| 14:O:70:PRO:O     | 14:O:72:HIS:CE1   | 2.64                     | 0.51              |
| 48:5:2297:G:C2    | 48:5:2338:C:N3    | 2.79                     | 0.51              |
| 48:5:1835:G:O2'   | 48:5:1836:G:OP2   | 2.21                     | 0.51              |
| 48:5:4913:G:O2'   | 48:5:4914:C:O4'   | 2.28                     | 0.51              |
| 48:5:476:G:N2     | 48:5:679:C:C2     | 2.79                     | 0.51              |
| 51:9:1784:G:N2    | 51:9:1785:C:C2    | 2.79                     | 0.51              |
| 2:B:378:ARG:HE    | 22:W:32:LEU:HD21  | 1.75                     | 0.51              |
| 8:H:111:LEU:HD11  | 8:H:125:ARG:HB2   | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:1139:C:H2'   | 51:9:1140:G:O4'    | 2.11                     | 0.51              |
| 48:5:77:U:C4      | 48:5:335:A:N1      | 2.76                     | 0.51              |
| 48:5:3723:A:C2    | 48:5:3724:A:C5     | 2.99                     | 0.51              |
| 2:B:252:ALA:HB3   | 48:5:4457:U:O2     | 2.10                     | 0.51              |
| 51:9:1303:C:O2    | 51:9:1303:C:O4'    | 2.24                     | 0.51              |
| 50:8:106:G:N2     | 50:8:107:C:C2      | 2.79                     | 0.51              |
| 48:5:5026:U:H3'   | 60:II:79:ILE:HD11  | 1.93                     | 0.51              |
| 51:9:211:G:N2     | 51:9:212:C:C2      | 2.78                     | 0.51              |
| 48:5:4093:G:C3'   | 48:5:4094:G:H5'    | 2.41                     | 0.51              |
| 51:9:88:G:C6      | 51:9:89:C:C4       | 2.99                     | 0.51              |
| 74:WW:81:VAL:HG11 | 74:WW:86:LEU:HD13  | 1.92                     | 0.51              |
| 70:SS:86:ARG:HB2  | 70:SS:98:VAL:HG23  | 1.93                     | 0.51              |
| 25:Z:5:MET:HG2    | 25:Z:77:TYR:CE1    | 2.46                     | 0.51              |
| 48:5:2768:C:O4'   | 48:5:2768:C:O2     | 2.26                     | 0.51              |
| 48:5:3628:G:C2    | 48:5:3834:C:C2     | 2.98                     | 0.51              |
| 67:PP:20:VAL:HG13 | 67:PP:24:GLN:HG2   | 1.93                     | 0.51              |
| 51:9:1735:A:H2'   | 51:9:1736:G:O4'    | 2.11                     | 0.51              |
| 51:9:379:C:O2     | 60:II:5:ARG:HD2    | 2.11                     | 0.51              |
| 48:5:3782:C:C2    | 48:5:3811:G:N2     | 2.79                     | 0.51              |
| 2:B:340:THR:OG1   | 2:B:341:LYS:N      | 2.43                     | 0.51              |
| 3:C:334:THR:HG21  | 6:F:53:TYR:OH      | 2.11                     | 0.51              |
| 48:5:1358:G:C2'   | 48:5:1359:G:O4'    | 2.59                     | 0.51              |
| 56:EE:122:LYS:HB3 | 56:EE:164:LEU:HD21 | 1.93                     | 0.51              |
| 48:5:1400:G:C6    | 48:5:1401:C:C4     | 2.99                     | 0.51              |
| 2:B:302:ASN:HB2   | 2:B:313:SER:HA     | 1.93                     | 0.51              |
| 23:X:76:ILE:HG21  | 23:X:112:ALA:HB2   | 1.91                     | 0.50              |
| 51:9:384:U:O2'    | 63:LL:135:SER:C    | 2.50                     | 0.50              |
| 48:5:4758:U:O4'   | 48:5:4758:U:O2     | 2.29                     | 0.50              |
| 48:5:4303:C:O4'   | 48:5:4303:C:O2     | 2.26                     | 0.50              |
| 51:9:1537:A:C2    | 51:9:1596:U:N3     | 2.79                     | 0.50              |
| 21:V:82:ILE:HD12  | 21:V:104:VAL:HG22  | 1.93                     | 0.50              |
| 9:I:97:ILE:HD13   | 9:I:126:VAL:HG11   | 1.92                     | 0.50              |
| 51:9:151:C:O2'    | 58:GG:132:ARG:NH1  | 2.43                     | 0.50              |
| 51:9:56:G:OP1     | 76:YY:111:LYS:NZ   | 2.31                     | 0.50              |
| 47:3:1:G:N1       | 47:3:2:C:C4        | 2.80                     | 0.50              |
| 48:5:2712:G:N2    | 48:5:2713:C:C2     | 2.79                     | 0.50              |
| 48:5:4389:C:H2'   | 48:5:4390:A:H8     | 1.76                     | 0.50              |
| 48:5:4906:C:C2    | 48:5:4916:G:C2     | 2.99                     | 0.50              |
| 48:5:929:A:H3'    | 48:5:930:G:C5'     | 2.40                     | 0.50              |
| 55:DD:191:PRO:O   | 55:DD:193:ASP:N    | 2.45                     | 0.50              |
| 25:Z:15:ALA:HB3   | 25:Z:79:HIS:HB3    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:504:G:C2      | 48:5:654:C:C2      | 2.99                     | 0.50              |
| 48:5:3717:A:N1     | 48:5:3933:G:H1'    | 2.26                     | 0.50              |
| 48:5:4583:C:N4     | 48:5:4718:G:C6     | 2.80                     | 0.50              |
| 51:9:501:C:C2'     | 51:9:501:C:O2      | 2.58                     | 0.50              |
| 52:AA:134:LEU:HD21 | 52:AA:144:THR:HG21 | 1.93                     | 0.50              |
| 51:9:407:G:N3      | 51:9:407:G:H2'     | 2.26                     | 0.50              |
| 51:9:1739:C:C2     | 51:9:1796:G:C2     | 3.00                     | 0.50              |
| 51:9:1207:G:C6     | 51:9:1837:G:C6     | 2.99                     | 0.50              |
| 51:9:1666:C:H2'    | 51:9:1667:U:O4'    | 2.11                     | 0.50              |
| 7:G:95:LEU:HD13    | 7:G:184:LEU:HD11   | 1.93                     | 0.50              |
| 48:5:2028:C:O2'    | 48:5:2029:A:O4'    | 2.29                     | 0.50              |
| 48:5:1214:C:H1'    | 48:5:1215:C:OP2    | 2.10                     | 0.50              |
| 48:5:1265:G:C2'    | 48:5:1266:G:H5'    | 2.41                     | 0.50              |
| 46:2:53:G:N2       | 46:2:62:C:C2       | 2.79                     | 0.50              |
| 48:5:4966:A:C2     | 48:5:4967:A:C2     | 2.99                     | 0.50              |
| 10:J:156:ARG:NH2   | 49:7:17:C:OP1      | 2.44                     | 0.50              |
| 51:9:1587:G:N2     | 71:TT:74:SER:OG    | 2.45                     | 0.50              |
| 51:9:1364:U:O4'    | 51:9:1364:U:O2     | 2.28                     | 0.50              |
| 48:5:1072:C:O2     | 48:5:1072:C:C2'    | 2.60                     | 0.50              |
| 14:O:54:TYR:CE1    | 14:O:145:VAL:HG11  | 2.47                     | 0.50              |
| 48:5:105:A:C2      | 48:5:336:A:C8      | 3.00                     | 0.50              |
| 51:9:1386:A:HO2'   | 51:9:1387:G:H5'    | 1.75                     | 0.50              |
| 51:9:598:G:N2      | 51:9:639:C:C2      | 2.79                     | 0.50              |
| 51:9:290:U:OP1     | 56:EE:156:MET:CE   | 2.60                     | 0.50              |
| 12:M:69:ARG:O      | 12:M:71:LYS:N      | 2.42                     | 0.50              |
| 2:B:43:LEU:HD13    | 2:B:196:TRP:CH2    | 2.46                     | 0.50              |
| 48:5:2627:C:O2     | 48:5:2627:C:O4'    | 2.30                     | 0.50              |
| 50:8:125:C:O4'     | 50:8:125:C:O2      | 2.29                     | 0.50              |
| 51:9:1116:C:O2     | 51:9:1116:C:O4'    | 2.28                     | 0.50              |
| 48:5:4462:C:C2     | 48:5:4515:G:C2     | 3.00                     | 0.50              |
| 51:9:155:G:N2      | 58:GG:56:ASN:OD1   | 2.45                     | 0.50              |
| 48:5:4281:A:C2     | 48:5:4283:G:C6     | 2.99                     | 0.50              |
| 48:5:1263:A:C6     | 48:5:1264:C:C4     | 3.00                     | 0.50              |
| 48:5:2090:U:OP2    | 48:5:2090:U:O4'    | 2.30                     | 0.50              |
| 58:GG:5:ILE:HG12   | 58:GG:111:LEU:HD12 | 1.94                     | 0.50              |
| 48:5:93:G:O2'      | 48:5:94:A:O4'      | 2.25                     | 0.50              |
| 51:9:350:C:O2'     | 51:9:383:G:N1      | 2.43                     | 0.50              |
| 68:QQ:52:LEU:HD13  | 68:QQ:56:LEU:HD21  | 1.94                     | 0.50              |
| 53:BB:150:ILE:O    | 53:BB:150:ILE:HG23 | 2.11                     | 0.50              |
| 47:3:31:A:H2'      | 57:FF:136:ARG:HH22 | 1.77                     | 0.50              |
| 48:5:1171:G:C2     | 48:5:1191:C:C2     | 2.99                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1622:U:C6     | 70:SS:120:HIS:CE1  | 3.00                     | 0.50              |
| 48:5:1983:A:C2     | 48:5:2010:A:H5''   | 2.47                     | 0.50              |
| 51:9:1681:U:O2'    | 51:9:1682:C:C5'    | 2.60                     | 0.50              |
| 51:9:92:A:O4'      | 56:EE:3:ARG:NH1    | 2.45                     | 0.50              |
| 48:5:1399:G:H2'    | 48:5:1400:G:O4'    | 2.12                     | 0.50              |
| 48:5:2123:C:O2'    | 48:5:2124:G:OP2    | 2.20                     | 0.50              |
| 51:9:970:G:H3'     | 51:9:971:G:C5'     | 2.41                     | 0.50              |
| 63:LL:11:GLN:HB3   | 63:LL:56:ILE:HD11  | 1.94                     | 0.50              |
| 2:B:220:ILE:HG12   | 2:B:278:THR:HG23   | 1.93                     | 0.50              |
| 56:EE:87:MET:CE    | 56:EE:236:ILE:HD13 | 2.42                     | 0.50              |
| 48:5:4213:A:N6     | 48:5:4218:U:H3     | 2.10                     | 0.50              |
| 48:5:1381:U:O2     | 48:5:1381:U:O4'    | 2.28                     | 0.50              |
| 48:5:1998:A:O2'    | 48:5:1999:A:O4'    | 2.30                     | 0.50              |
| 51:9:474:G:N1      | 51:9:475:C:C4      | 2.80                     | 0.50              |
| 51:9:88:G:C2       | 51:9:89:C:C2       | 3.00                     | 0.50              |
| 48:5:1910:G:N2     | 48:5:1911:C:C2     | 2.80                     | 0.50              |
| 60:II:76:THR:HG21  | 60:II:105:ASP:O    | 2.12                     | 0.50              |
| 9:I:181:PHE:O      | 9:I:185:VAL:HG23   | 2.12                     | 0.50              |
| 56:EE:131:VAL:HA   | 56:EE:137:PRO:HA   | 1.94                     | 0.50              |
| 49:7:71:G:C2       | 49:7:105:C:C2      | 3.00                     | 0.50              |
| 48:5:1235:G:H2'    | 48:5:1236:C:H5'    | 1.93                     | 0.50              |
| 51:9:193:C:C2      | 51:9:207:G:C2      | 2.99                     | 0.50              |
| 48:5:1167:C:C2     | 48:5:1195:G:C2     | 3.00                     | 0.50              |
| 66:OO:44:VAL:HG11  | 66:OO:85:CYS:SG    | 2.52                     | 0.50              |
| 48:5:2368:A:N6     | 48:5:2788:U:O2     | 2.45                     | 0.50              |
| 70:SS:11:HIS:O     | 70:SS:12:ILE:CD1   | 2.52                     | 0.50              |
| 48:5:2028:C:O2'    | 48:5:2029:A:C5'    | 2.60                     | 0.50              |
| 61:JJ:38:ARG:HG2   | 61:JJ:38:ARG:O     | 2.12                     | 0.50              |
| 48:5:4094:G:H2'    | 48:5:4095:G:O4'    | 2.12                     | 0.50              |
| 17:R:109:TYR:HB3   | 17:R:115:ILE:HG12  | 1.94                     | 0.50              |
| 5:E:134:ARG:NH1    | 5:E:165:SER:O      | 2.45                     | 0.50              |
| 48:5:5031:G:N2     | 48:5:5032:C:C2     | 2.80                     | 0.50              |
| 48:5:3715:U:O2'    | 48:5:3716:C:O4'    | 2.28                     | 0.50              |
| 48:5:2752:G:H2'    | 48:5:2753:G:O4'    | 2.12                     | 0.50              |
| 48:5:1811:G:N2     | 48:5:1812:C:C2     | 2.80                     | 0.50              |
| 48:5:975:C:C3'     | 48:5:976:G:O4'     | 2.60                     | 0.49              |
| 48:5:166:C:C2      | 48:5:167:C:H5      | 2.30                     | 0.49              |
| 48:5:1400:G:C2     | 48:5:1401:C:C2     | 3.00                     | 0.49              |
| 71:TT:75:MET:HA    | 71:TT:78:ILE:HG22  | 1.93                     | 0.49              |
| 48:5:2311:C:C2     | 48:5:2328:G:C2     | 3.00                     | 0.49              |
| 54:CC:107:LEU:HD11 | 54:CC:129:ALA:HB2  | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1886:G:C2     | 48:5:1894:C:C2     | 3.00                     | 0.49              |
| 48:5:2463:G:N2     | 48:5:2464:C:C2     | 2.80                     | 0.49              |
| 2:B:241:PRO:O      | 2:B:244:THR:OG1    | 2.30                     | 0.49              |
| 48:5:1956:A:HO2'   | 48:5:1957:U:H5'    | 1.76                     | 0.49              |
| 51:9:92:A:C6       | 51:9:446:G:C6      | 3.00                     | 0.49              |
| 11:L:65:ARG:HG2    | 11:L:66:TYR:CD2    | 2.48                     | 0.49              |
| 48:5:1872:G:O2'    | 48:5:4219:A:N3     | 2.38                     | 0.49              |
| 48:5:2588:C:OP1    | 48:5:2767:U:O2'    | 2.30                     | 0.49              |
| 48:5:1776:A:C6     | 48:5:1777:C:C4     | 2.99                     | 0.49              |
| 53:BB:137:LEU:HD23 | 53:BB:215:VAL:HG22 | 1.94                     | 0.49              |
| 51:9:182:C:H2'     | 51:9:184:G:H1'     | 1.93                     | 0.49              |
| 5:E:208:LEU:HD12   | 5:E:208:LEU:O      | 2.12                     | 0.49              |
| 47:3:66:U:H2'      | 47:3:67:U:O4'      | 2.11                     | 0.49              |
| 56:EE:153:LEU:HD11 | 58:GG:216:ARG:NE   | 2.28                     | 0.49              |
| 9:I:76:MET:HG3     | 9:I:87:ILE:HD11    | 1.93                     | 0.49              |
| 51:9:1401:A:C2     | 51:9:1402:A:N1     | 2.81                     | 0.49              |
| 48:5:2257:C:O2'    | 48:5:2258:C:O5'    | 2.25                     | 0.49              |
| 1:A:49:ILE:HG22    | 1:A:58:LEU:HB2     | 1.94                     | 0.49              |
| 51:9:887:U:O4'     | 51:9:887:U:O2      | 2.29                     | 0.49              |
| 56:EE:15:PRO:HD2   | 56:EE:18:TRP:CZ3   | 2.47                     | 0.49              |
| 48:5:1412:G:N2     | 48:5:1413:C:C2     | 2.79                     | 0.49              |
| 48:5:230:G:C2      | 48:5:239:C:C2      | 3.01                     | 0.49              |
| 17:R:105:LEU:HD12  | 17:R:138:LEU:HD13  | 1.94                     | 0.49              |
| 48:5:3752:C:H2'    | 48:5:3777:G:C8     | 2.47                     | 0.49              |
| 51:9:666:U:H2'     | 51:9:667:U:C6      | 2.47                     | 0.49              |
| 48:5:1245:C:C4     | 48:5:1269:G:O6     | 2.66                     | 0.49              |
| 48:5:4579:U:O2     | 48:5:4580:U:C2     | 2.65                     | 0.49              |
| 48:5:2108:G:N2     | 48:5:2125:C:C2     | 2.80                     | 0.49              |
| 48:5:93:G:H2'      | 48:5:94:A:C8       | 2.48                     | 0.49              |
| 48:5:2336:G:C2     | 48:5:2337:C:C2     | 3.01                     | 0.49              |
| 13:N:67:ARG:NH1    | 48:5:2458:C:OP1    | 2.45                     | 0.49              |
| 61:JJ:46:VAL:HG11  | 61:JJ:106:LEU:HD12 | 1.94                     | 0.49              |
| 48:5:356:G:O2'     | 50:8:25:G:N3       | 2.44                     | 0.49              |
| 51:9:1408:U:H2'    | 51:9:1409:A:C8     | 2.47                     | 0.49              |
| 48:5:1297:U:O4'    | 48:5:1297:U:P      | 2.71                     | 0.49              |
| 61:JJ:28:GLU:HB3   | 61:JJ:40:LYS:HD2   | 1.94                     | 0.49              |
| 3:C:213:GLU:OE1    | 3:C:213:GLU:N      | 2.46                     | 0.49              |
| 51:9:73:C:O4'      | 51:9:73:C:O2       | 2.28                     | 0.49              |
| 48:5:325:U:H2'     | 48:5:326:C:C6      | 2.47                     | 0.49              |
| 48:5:1613:A:C2     | 48:5:1630:A:C2     | 3.00                     | 0.49              |
| 15:P:54:GLN:HA     | 15:P:83:TRP:CD1    | 2.47                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:9:1481:G:C6    | 51:9:1482:C:N3     | 2.80                     | 0.49              |
| 48:5:1960:A:H4'   | 48:5:1961:G:OP2    | 2.11                     | 0.49              |
| 48:5:1269:G:C5    | 48:5:2111:G:C2     | 3.01                     | 0.49              |
| 48:5:4411:G:C2    | 48:5:4432:C:O2     | 2.65                     | 0.49              |
| 48:5:300:A:C2     | 48:5:301:G:C6      | 3.01                     | 0.49              |
| 48:5:2494:U:H2'   | 48:5:2495:U:O4'    | 2.12                     | 0.49              |
| 9:I:14:ASN:O      | 9:I:128:ARG:NH2    | 2.45                     | 0.49              |
| 48:5:2519:U:C2    | 48:5:2520:C:C5     | 3.01                     | 0.49              |
| 4:D:258:LYS:O     | 4:D:259:ARG:HG3    | 2.13                     | 0.49              |
| 51:9:1511:U:H2'   | 51:9:1512:C:C6     | 2.48                     | 0.49              |
| 9:I:46:PHE:CD1    | 9:I:140:THR:HA     | 2.48                     | 0.49              |
| 12:M:24:LEU:HD11  | 12:M:86:TRP:CG     | 2.47                     | 0.49              |
| 4:D:200:MET:HE1   | 4:D:241:LYS:HG2    | 1.93                     | 0.49              |
| 48:5:2557:G:C6    | 48:5:2558:C:C4     | 3.01                     | 0.49              |
| 65:NN:60:VAL:HG23 | 65:NN:66:VAL:HG21  | 1.93                     | 0.49              |
| 48:5:3782:C:N3    | 48:5:3811:G:C2     | 2.81                     | 0.49              |
| 48:5:2056:G:C8    | 48:5:2058:G:C8     | 3.00                     | 0.49              |
| 48:5:3626:G:C6    | 48:5:3836:A:C2     | 3.01                     | 0.49              |
| 48:5:2726:G:C6    | 48:5:2727:C:N4     | 2.81                     | 0.49              |
| 48:5:1170:G:C2    | 48:5:1192:C:C2     | 3.00                     | 0.49              |
| 48:5:1726:U:H3    | 48:5:1836:G:H1     | 1.61                     | 0.49              |
| 48:5:4489:G:C6    | 48:5:4490:C:C4     | 3.00                     | 0.49              |
| 48:5:1301:C:O4'   | 48:5:1301:C:O2     | 2.29                     | 0.49              |
| 20:U:80:LYS:HD3   | 20:U:110:TYR:CE2   | 2.47                     | 0.49              |
| 51:9:1654:G:N2    | 51:9:1655:C:C2     | 2.81                     | 0.49              |
| 74:WW:90:GLN:HA   | 74:WW:102:ILE:HD11 | 1.93                     | 0.49              |
| 48:5:4574:U:H3'   | 48:5:4575:G:H5"    | 1.94                     | 0.49              |
| 48:5:4079:C:C2    | 48:5:4168:G:C2     | 3.01                     | 0.49              |
| 48:5:977:C:H2'    | 48:5:978:G:O4'     | 2.12                     | 0.49              |
| 5:E:254:LEU:N     | 5:E:255:PRO:HD2    | 2.28                     | 0.49              |
| 47:3:35:U:H1'     | 51:9:1641:A:P      | 2.53                     | 0.49              |
| 48:5:986:C:N3     | 48:5:1068:G:C2     | 2.81                     | 0.49              |
| 11:L:66:TYR:O     | 11:L:68:THR:N      | 2.46                     | 0.49              |
| 48:5:1400:G:H2'   | 48:5:1401:C:O4'    | 2.13                     | 0.49              |
| 48:5:4735:G:C6    | 48:5:4736:C:C4     | 3.01                     | 0.49              |
| 48:5:4913:G:HO2'  | 48:5:4914:C:C1'    | 2.24                     | 0.49              |
| 16:Q:86:ILE:HB    | 16:Q:105:VAL:HG13  | 1.95                     | 0.49              |
| 51:9:123:G:C2     | 51:9:342:C:C2      | 3.01                     | 0.49              |
| 48:5:384:A:C6     | 48:5:386:A:C6      | 3.01                     | 0.49              |
| 1:A:107:MET:SD    | 1:A:113:VAL:HG11   | 2.53                     | 0.49              |
| 48:5:224:U:O2     | 48:5:224:U:O4'     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:1754:U:O4'   | 48:5:1754:U:O2    | 2.30                     | 0.49              |
| 1:A:44:ILE:HG22   | 1:A:87:PHE:CD2    | 2.48                     | 0.49              |
| 48:5:1328:G:O2'   | 48:5:2349:A:OP1   | 2.31                     | 0.49              |
| 51:9:635:G:C6     | 51:9:636:C:C4     | 3.01                     | 0.49              |
| 48:5:4932:U:H2'   | 48:5:4933:C:O4'   | 2.13                     | 0.49              |
| 48:5:4691:A:C2    | 48:5:4700:A:C4    | 3.00                     | 0.49              |
| 48:5:956:A:H3'    | 48:5:957:G:C8     | 2.48                     | 0.49              |
| 51:9:1406:G:C5    | 51:9:1407:U:H1'   | 2.47                     | 0.49              |
| 51:9:1212:G:C2    | 51:9:1213:C:C2    | 3.01                     | 0.49              |
| 48:5:2557:G:C2    | 48:5:2558:C:C2    | 3.01                     | 0.49              |
| 52:AA:42:LYS:HG2  | 52:AA:48:ILE:HD11 | 1.95                     | 0.49              |
| 2:B:165:HIS:HB3   | 2:B:180:LEU:HG    | 1.95                     | 0.49              |
| 51:9:1315:U:O2    | 51:9:1315:U:O4'   | 2.29                     | 0.49              |
| 57:FF:76:MET:HA   | 57:FF:155:CYS:SG  | 2.53                     | 0.49              |
| 4:D:195:HIS:CE1   | 4:D:199:ILE:HD11  | 2.48                     | 0.49              |
| 47:3:24:G:C6      | 47:3:25:C:C4      | 3.01                     | 0.49              |
| 48:5:2730:U:H2'   | 48:5:2731:C:C6    | 2.48                     | 0.49              |
| 48:5:1252:C:C2    | 48:5:1259:G:C2    | 3.01                     | 0.49              |
| 48:5:3724:A:N6    | 48:5:3725:G:C6    | 2.81                     | 0.48              |
| 51:9:1444:U:O2'   | 51:9:1580:A:N1    | 2.45                     | 0.48              |
| 51:9:958:G:C2     | 51:9:959:G:C6     | 3.01                     | 0.48              |
| 48:5:5020:G:H2'   | 48:5:5021:C:O4'   | 2.13                     | 0.48              |
| 51:9:1411:G:H3'   | 51:9:1412:C:H4'   | 1.94                     | 0.48              |
| 57:FF:20:PHE:CZ   | 57:FF:69:VAL:HG11 | 2.47                     | 0.48              |
| 16:Q:11:ARG:NH2   | 48:5:1690:C:OP2   | 2.46                     | 0.48              |
| 17:R:172:ARG:HH12 | 51:9:908:A:C5'    | 1.81                     | 0.48              |
| 47:3:6:G:N1       | 47:3:7:A:C5       | 2.81                     | 0.48              |
| 48:5:1279:A:O2'   | 48:5:1280:C:OP1   | 2.30                     | 0.48              |
| 47:3:34:U:O2'     | 47:3:35:U:O4'     | 2.31                     | 0.48              |
| 51:9:409:C:N3     | 51:9:432:G:C2     | 2.81                     | 0.48              |
| 47:3:10:G:N1      | 47:3:11:C:C4      | 2.81                     | 0.48              |
| 48:5:1449:C:H2'   | 48:5:1450:C:O4'   | 2.12                     | 0.48              |
| 48:5:4099:G:C6    | 48:5:4100:C:C4    | 3.01                     | 0.48              |
| 52:AA:66:VAL:HG11 | 73:VV:46:PHE:HB2  | 1.95                     | 0.48              |
| 48:5:4129:G:H2'   | 48:5:4130:C:O4'   | 2.14                     | 0.48              |
| 16:Q:186:TYR:CD2  | 48:5:4307:A:H4'   | 2.48                     | 0.48              |
| 51:9:916:A:C5     | 65:NN:73:ARG:HD3  | 2.48                     | 0.48              |
| 48:5:990:C:C4     | 48:5:1064:G:C2    | 3.01                     | 0.48              |
| 48:5:4213:A:C2    | 48:5:4218:U:O4    | 2.57                     | 0.48              |
| 48:5:2468:U:O2    | 48:5:2469:C:C5    | 2.66                     | 0.48              |
| 48:5:2027:U:HO2'  | 48:5:2028:C:H5'   | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:919:C:N4     | 48:5:920:C:N4     | 2.61                     | 0.48              |
| 76:YY:113:ARG:O   | 76:YY:114:MET:CB  | 2.61                     | 0.48              |
| 48:5:671:G:C2     | 48:5:672:C:C2     | 3.01                     | 0.48              |
| 4:D:3:PHE:HB2     | 48:5:1755:C:C6    | 2.48                     | 0.48              |
| 3:C:303:ARG:O     | 16:Q:38:ARG:NH1   | 2.42                     | 0.48              |
| 69:RR:91:LEU:HD12 | 69:RR:92:ASP:N    | 2.28                     | 0.48              |
| 51:9:114:G:N7     | 63:LL:69:ARG:NH1  | 2.60                     | 0.48              |
| 48:5:4724:A:C6    | 48:5:4725:C:C4    | 3.01                     | 0.48              |
| 51:9:1212:G:HO2'  | 51:9:1213:C:C5'   | 2.24                     | 0.48              |
| 48:5:100:C:H2'    | 48:5:101:A:O4'    | 2.13                     | 0.48              |
| 48:5:125:C:O2'    | 48:5:126:C:OP1    | 2.22                     | 0.48              |
| 48:5:505:G:C2     | 48:5:506:C:C2     | 3.01                     | 0.48              |
| 51:9:17:C:O2'     | 51:9:1194:A:N1    | 2.36                     | 0.48              |
| 51:9:830:A:C6     | 51:9:844:U:N3     | 2.82                     | 0.48              |
| 51:9:1408:U:C4    | 51:9:1409:A:C6    | 3.01                     | 0.48              |
| 51:9:217:A:C2     | 51:9:309:G:C6     | 3.01                     | 0.48              |
| 51:9:1617:G:N1    | 51:9:1620:A:OP2   | 2.45                     | 0.48              |
| 51:9:1380:C:H2'   | 51:9:1381:G:O4'   | 2.13                     | 0.48              |
| 48:5:1448:G:N2    | 48:5:1449:C:C2    | 2.81                     | 0.48              |
| 48:5:2539:C:H2'   | 48:5:2540:C:C6    | 2.48                     | 0.48              |
| 2:B:234:ARG:HA    | 2:B:272:LYS:HD2   | 1.95                     | 0.48              |
| 64:MM:113:ASP:O   | 64:MM:115:GLY:N   | 2.47                     | 0.48              |
| 13:N:65:ARG:HG3   | 13:N:129:PHE:CE1  | 2.49                     | 0.48              |
| 20:U:100:LEU:HD22 | 20:U:112:LEU:HB3  | 1.96                     | 0.48              |
| 48:5:4136:G:C6    | 48:5:4137:C:C4    | 3.01                     | 0.48              |
| 61:JJ:45:ARG:O    | 61:JJ:49:THR:HG23 | 2.14                     | 0.48              |
| 7:G:32:PHE:CZ     | 25:Z:55:ALA:HA    | 2.48                     | 0.48              |
| 48:5:2336:G:C6    | 48:5:2337:C:C4    | 3.02                     | 0.48              |
| 48:5:2729:C:H2'   | 48:5:2730:U:O4'   | 2.13                     | 0.48              |
| 51:9:1321:G:H2'   | 51:9:1322:G:O4'   | 2.14                     | 0.48              |
| 48:5:3896:C:O2    | 48:5:4564:A:N1    | 2.46                     | 0.48              |
| 48:5:965:G:N3     | 48:5:965:G:H2'    | 2.29                     | 0.48              |
| 48:5:4989:U:O2    | 48:5:4989:U:O4'   | 2.30                     | 0.48              |
| 48:5:4767:C:C2    | 48:5:4868:G:C2    | 3.01                     | 0.48              |
| 48:5:3586:G:C6    | 48:5:3587:C:C4    | 3.02                     | 0.48              |
| 48:5:28:C:C2      | 48:5:55:G:C2      | 3.02                     | 0.48              |
| 48:5:2468:U:C4    | 48:5:2473:A:N6    | 2.77                     | 0.48              |
| 47:3:68:C:H2'     | 47:3:69:G:C8      | 2.48                     | 0.48              |
| 48:5:1983:A:C2    | 48:5:2008:U:O4    | 2.65                     | 0.48              |
| 51:9:1466:G:C2    | 51:9:1467:C:C4    | 3.02                     | 0.48              |
| 51:9:841:G:C2     | 51:9:842:C:C2     | 3.01                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:1942:A:N3    | 48:5:4432:C:O2'    | 2.44                     | 0.48              |
| 57:FF:68:ILE:HD12 | 57:FF:112:LEU:HD22 | 1.94                     | 0.48              |
| 48:5:1910:G:C6    | 48:5:1911:C:N4     | 2.82                     | 0.48              |
| 54:CC:129:ALA:HB2 | 54:CC:213:LEU:HD11 | 1.95                     | 0.48              |
| 48:5:2909:C:C2    | 48:5:3586:G:C2     | 3.01                     | 0.48              |
| 48:5:2496:G:C2    | 48:5:2497:C:C2     | 3.02                     | 0.48              |
| 48:5:2844:A:O2'   | 48:5:4631:G:H4'    | 2.14                     | 0.48              |
| 12:M:36:ALA:HB2   | 12:M:52:PHE:CE1    | 2.49                     | 0.48              |
| 48:5:1383:G:C5    | 48:5:1384:C:C4     | 3.02                     | 0.48              |
| 48:5:1308:C:H2'   | 48:5:1309:C:C6     | 2.49                     | 0.48              |
| 13:N:124:ASP:OD1  | 13:N:125:SER:N     | 2.46                     | 0.48              |
| 51:9:629:A:N6     | 51:9:632:C:C2      | 2.82                     | 0.48              |
| 51:9:322:C:O2     | 51:9:323:C:C6      | 2.66                     | 0.48              |
| 5:E:254:LEU:O     | 5:E:257:ILE:HG12   | 2.14                     | 0.48              |
| 51:9:830:A:N6     | 51:9:844:U:C2      | 2.81                     | 0.48              |
| 51:9:1235:G:C5'   | 51:9:1247:C:N4     | 2.75                     | 0.48              |
| 51:9:516:A:N1     | 51:9:643:A:O2'     | 2.44                     | 0.48              |
| 51:9:1771:G:N1    | 51:9:1772:C:C4     | 2.82                     | 0.48              |
| 48:5:3860:A:H61   | 48:5:4560:C:H5     | 1.61                     | 0.48              |
| 51:9:1333:U:H4'   | 55:DD:147:ALA:HB2  | 1.95                     | 0.48              |
| 51:9:191:A:H3'    | 51:9:192:C:H5''    | 1.95                     | 0.48              |
| 16:Q:67:ILE:HD12  | 16:Q:96:PRO:HD2    | 1.96                     | 0.48              |
| 48:5:2477:A:H2'   | 48:5:2478:C:C6     | 2.48                     | 0.48              |
| 52:AA:63:ARG:HG2  | 52:AA:185:MET:HE1  | 1.96                     | 0.48              |
| 48:5:1956:A:C2'   | 48:5:1957:U:H5'    | 2.43                     | 0.48              |
| 48:5:1878:G:N2    | 48:5:1879:C:C2     | 2.81                     | 0.48              |
| 67:PP:22:LEU:HA   | 67:PP:25:LEU:HB2   | 1.95                     | 0.48              |
| 48:5:3714:G:C6    | 48:5:3715:U:C4     | 3.02                     | 0.48              |
| 48:5:5020:G:C2    | 48:5:5021:C:C2     | 3.02                     | 0.48              |
| 68:QQ:44:PRO:HG2  | 68:QQ:81:ILE:HD11  | 1.95                     | 0.48              |
| 4:D:146:LEU:HD11  | 4:D:159:VAL:HG11   | 1.94                     | 0.48              |
| 48:5:80:C:C2      | 48:5:104:G:C2      | 3.01                     | 0.48              |
| 48:5:484:U:C4     | 48:5:486:C:C5      | 3.02                     | 0.48              |
| 51:9:1149:A:O2'   | 51:9:1150:A:H3'    | 2.14                     | 0.48              |
| 48:5:1699:A:N6    | 48:5:2094:G:O2'    | 2.46                     | 0.48              |
| 51:9:506:G:OP1    | 76:YY:108:LYS:NZ   | 2.44                     | 0.48              |
| 51:9:99:A:H2'     | 51:9:100:U:O4'     | 2.13                     | 0.48              |
| 48:5:3712:A:C2    | 51:9:970:G:C6      | 3.02                     | 0.48              |
| 48:5:3715:U:H2'   | 48:5:3716:C:C6     | 2.48                     | 0.48              |
| 48:5:351:C:C2     | 50:8:25:G:N2       | 2.82                     | 0.48              |
| 9:I:45:GLU:O      | 9:I:46:PHE:CD1     | 2.67                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 48:5:2814:C:C2'  | 48:5:2814:C:O2    | 2.62                     | 0.48              |
| 2:B:105:VAL:HG11 | 2:B:150:PHE:CZ    | 2.49                     | 0.48              |
| 48:5:984:C:C2    | 48:5:1070:G:C2    | 3.01                     | 0.48              |
| 5:E:254:LEU:O    | 5:E:258:LYS:HG3   | 2.13                     | 0.47              |
| 51:9:830:A:H2'   | 51:9:831:G:O4'    | 2.13                     | 0.47              |
| 48:5:1987:C:C2'  | 48:5:1987:C:O2    | 2.61                     | 0.47              |
| 48:5:1075:G:C2   | 48:5:1076:C:C2    | 3.02                     | 0.47              |
| 48:5:505:G:C6    | 48:5:506:C:C4     | 3.02                     | 0.47              |
| 48:5:2496:G:C6   | 48:5:2497:C:C4    | 3.02                     | 0.47              |
| 8:H:39:ASN:O     | 8:H:40:HIS:HB3    | 2.14                     | 0.47              |
| 51:9:62:G:O4'    | 51:9:172:U:N3     | 2.46                     | 0.47              |
| 51:9:185:G:N2    | 51:9:186:C:C2     | 2.82                     | 0.47              |
| 48:5:508:G:C2    | 48:5:510:U:C5     | 3.02                     | 0.47              |
| 51:9:491:C:H2'   | 51:9:492:C:O4'    | 2.14                     | 0.47              |
| 11:L:74:ARG:NH2  | 48:5:76:A:N7      | 2.63                     | 0.47              |
| 48:5:1279:A:H2'  | 48:5:1280:C:C6    | 2.49                     | 0.47              |
| 17:R:61:ALA:HB2  | 48:5:2633:U:H5''  | 1.96                     | 0.47              |
| 51:9:1537:A:H2'  | 51:9:1538:C:O4'   | 2.14                     | 0.47              |
| 51:9:1126:G:N2   | 51:9:1127:C:C2    | 2.83                     | 0.47              |
| 50:8:139:G:C6    | 50:8:140:C:C4     | 3.02                     | 0.47              |
| 48:5:1345:A:H2'  | 48:5:1346:C:C6    | 2.48                     | 0.47              |
| 48:5:1995:G:C2   | 48:5:1996:C:C2    | 3.02                     | 0.47              |
| 52:AA:109:THR:O  | 52:AA:110:ASN:HB2 | 2.13                     | 0.47              |
| 48:5:977:C:H2'   | 48:5:978:G:H5'    | 1.96                     | 0.47              |
| 48:5:1958:A:P    | 48:5:1958:A:H3'   | 2.54                     | 0.47              |
| 2:B:36:ASP:N     | 2:B:36:ASP:OD1    | 2.44                     | 0.47              |
| 48:5:499:G:N3    | 48:5:499:G:H2'    | 2.28                     | 0.47              |
| 48:5:497:G:C2    | 48:5:657:C:N3     | 2.82                     | 0.47              |
| 51:9:1530:U:H2'  | 51:9:1531:A:O4'   | 2.14                     | 0.47              |
| 51:9:1108:G:C2   | 51:9:1125:C:C2    | 3.01                     | 0.47              |
| 51:9:1868:U:N3   | 52:AA:98:PRO:O    | 44.39                    | 0.47              |
| 74:WW:89:TRP:CE3 | 74:WW:93:LEU:HD22 | 2.49                     | 0.47              |
| 14:O:84:VAL:HG11 | 14:O:102:LEU:HD22 | 1.96                     | 0.47              |
| 48:5:2618:G:N2   | 48:5:2720:C:C2    | 2.82                     | 0.47              |
| 48:5:120:A:H2'   | 48:5:149:A:N6     | 2.30                     | 0.47              |
| 48:5:4152:G:N2   | 48:5:4153:C:C2    | 2.82                     | 0.47              |
| 48:5:279:A:H3'   | 48:5:279:A:OP1    | 2.14                     | 0.47              |
| 5:E:202:VAL:HG12 | 5:E:256:LYS:HZ1   | 1.74                     | 0.47              |
| 47:3:70:G:H4'    | 48:5:3740:G:O2'   | 2.15                     | 0.47              |
| 48:5:1367:C:H2'  | 48:5:1367:C:O2    | 2.14                     | 0.47              |
| 4:D:64:ILE:HG13  | 4:D:105:LEU:HD21  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:1661:C:C2    | 48:5:2345:G:N1    | 2.82                     | 0.47              |
| 51:9:1834:A:N3    | 51:9:1834:A:C2'   | 2.77                     | 0.47              |
| 14:O:109:PRO:HB2  | 14:O:110:PRO:CD   | 2.43                     | 0.47              |
| 1:A:193:ARG:NH2   | 48:5:3685:C:OP1   | 2.47                     | 0.47              |
| 14:O:196:LEU:HB3  | 14:O:202:LEU:HD22 | 1.97                     | 0.47              |
| 66:OO:142:ARG:HG3 | 66:OO:143:LYS:N   | 2.30                     | 0.47              |
| 9:I:184:MET:HE1   | 9:I:190:LEU:CG    | 2.45                     | 0.47              |
| 50:8:56:G:C6      | 50:8:57:C:C4      | 3.02                     | 0.47              |
| 48:5:4378:A:O2'   | 48:5:4379:A:H2'   | 2.14                     | 0.47              |
| 48:5:3662:A:N6    | 48:5:3680:U:N3    | 2.57                     | 0.47              |
| 48:5:1468:C:C2    | 48:5:1498:G:N2    | 2.82                     | 0.47              |
| 48:5:1448:G:C6    | 48:5:1449:C:N4    | 2.82                     | 0.47              |
| 48:5:4093:G:H3'   | 48:5:4094:G:H5'   | 1.95                     | 0.47              |
| 51:9:1537:A:N1    | 51:9:1596:U:C4    | 2.83                     | 0.47              |
| 48:5:4916:G:C2    | 48:5:4917:C:C2    | 3.02                     | 0.47              |
| 51:9:1667:U:H2'   | 51:9:1668:U:C6    | 2.49                     | 0.47              |
| 48:5:4099:G:C2    | 48:5:4100:C:C2    | 3.02                     | 0.47              |
| 48:5:1189:G:C6    | 48:5:1190:C:C4    | 3.02                     | 0.47              |
| 48:5:298:G:N2     | 48:5:299:C:C2     | 2.83                     | 0.47              |
| 55:DD:162:ASP:N   | 55:DD:163:PRO:HD2 | 2.29                     | 0.47              |
| 2:B:312:LYS:HD2   | 2:B:370:THR:HG21  | 1.97                     | 0.47              |
| 67:PP:26:LEU:N    | 67:PP:28:MET:SD   | 2.87                     | 0.47              |
| 48:5:2661:U:HO2'  | 48:5:2662:G:P     | 2.37                     | 0.47              |
| 48:5:4246:G:N2    | 48:5:4263:C:C2    | 2.83                     | 0.47              |
| 48:5:971:U:H2'    | 48:5:972:C:H5'    | 1.95                     | 0.47              |
| 6:F:49:ARG:NH1    | 48:5:974:C:O3'    | 2.48                     | 0.47              |
| 51:9:1445:U:O4    | 51:9:1446:A:N6    | 2.47                     | 0.47              |
| 48:5:2297:G:C2    | 48:5:2338:C:C2    | 3.03                     | 0.47              |
| 51:9:635:G:C2     | 51:9:636:C:C2     | 3.03                     | 0.47              |
| 51:9:172:U:O2     | 51:9:172:U:C2'    | 2.61                     | 0.47              |
| 6:F:211:TRP:CD1   | 6:F:212:PRO:HD2   | 2.50                     | 0.47              |
| 3:C:181:LYS:HD2   | 48:5:2300:A:N1    | 2.29                     | 0.47              |
| 48:5:4119:C:O4'   | 48:5:4119:C:O2    | 2.30                     | 0.47              |
| 48:5:2097:U:O4'   | 48:5:2097:U:O2    | 2.33                     | 0.47              |
| 17:R:11:ALA:HB1   | 17:R:50:ILE:HD13  | 1.96                     | 0.47              |
| 4:D:76:CYS:SG     | 4:D:77:ALA:N      | 2.87                     | 0.47              |
| 51:9:1754:G:C6    | 51:9:1755:C:C4    | 3.03                     | 0.47              |
| 9:I:153:ARG:HA    | 9:I:165:ILE:HD11  | 1.96                     | 0.47              |
| 5:E:62:LYS:NZ     | 48:5:978:G:P      | 2.81                     | 0.47              |
| 5:E:123:SER:O     | 5:E:126:ARG:HG2   | 2.15                     | 0.47              |
| 61:JJ:118:GLY:O   | 61:JJ:120:ALA:N   | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1357:C:O2'    | 48:5:1358:G:O4'    | 2.29                     | 0.47              |
| 48:5:1358:G:H2'    | 48:5:1359:G:C8     | 2.50                     | 0.47              |
| 48:5:2586:G:C8     | 48:5:2770:C:H1'    | 2.49                     | 0.47              |
| 3:C:161:TYR:CD1    | 3:C:166:GLU:HB3    | 2.49                     | 0.47              |
| 4:D:200:MET:HE1    | 4:D:241:LYS:HE3    | 1.96                     | 0.47              |
| 48:5:499:G:C2      | 48:5:656:C:N3      | 2.82                     | 0.47              |
| 48:5:1270:A:H2'    | 48:5:1271:G:O5'    | 2.15                     | 0.47              |
| 48:5:2089:G:HO2'   | 48:5:2090:U:P      | 2.37                     | 0.47              |
| 48:5:2128:G:C6     | 48:5:2129:C:C4     | 3.03                     | 0.47              |
| 48:5:4092:G:C2     | 48:5:4158:C:C2     | 3.02                     | 0.47              |
| 48:5:4525:C:H2'    | 48:5:4526:U:O4'    | 2.15                     | 0.47              |
| 56:EE:195:ILE:O    | 56:EE:196:THR:HB   | 2.15                     | 0.47              |
| 48:5:4303:C:O2     | 48:5:4303:C:O5'    | 2.32                     | 0.47              |
| 48:5:384:A:N6      | 48:5:386:A:C6      | 2.83                     | 0.47              |
| 24:Y:52:ASP:OD1    | 24:Y:52:ASP:N      | 2.47                     | 0.47              |
| 3:C:290:SER:O      | 3:C:294:LYS:HG2    | 2.14                     | 0.47              |
| 58:GG:57:ASP:HA    | 58:GG:106:LEU:HD23 | 1.96                     | 0.47              |
| 48:5:1787:A:N3     | 48:5:4210:U:O2'    | 2.44                     | 0.47              |
| 48:5:1246:G:H2'    | 48:5:1247:U:O4'    | 2.14                     | 0.47              |
| 51:9:1115:U:O4'    | 51:9:1115:U:O2     | 2.31                     | 0.47              |
| 48:5:2020:U:H2'    | 48:5:2020:U:O2     | 2.14                     | 0.47              |
| 51:9:1541:G:C6     | 51:9:1542:C:C4     | 3.03                     | 0.47              |
| 48:5:2459:G:N2     | 48:5:2462:C:OP2    | 2.47                     | 0.47              |
| 17:R:44:LEU:HD22   | 17:R:49:LEU:HD12   | 1.96                     | 0.47              |
| 52:AA:104:THR:O    | 52:AA:107:THR:HG23 | 2.14                     | 0.47              |
| 48:5:3938:G:O6     | 48:5:4172:A:N1     | 2.48                     | 0.47              |
| 51:9:322:C:C2'     | 51:9:323:C:OP2     | 2.62                     | 0.47              |
| 48:5:4919:G:C2     | 48:5:4920:C:C2     | 3.02                     | 0.47              |
| 56:EE:126:VAL:HG13 | 56:EE:160:ILE:HD11 | 1.96                     | 0.47              |
| 48:5:4730:C:O5'    | 48:5:4731:G:N2     | 2.47                     | 0.47              |
| 48:5:4489:G:C2     | 48:5:4490:C:C2     | 3.02                     | 0.47              |
| 3:C:268:ARG:NH2    | 48:5:655:C:OP2     | 2.47                     | 0.47              |
| 51:9:1228:A:H2'    | 51:9:1229:G:C8     | 2.50                     | 0.47              |
| 48:5:2907:G:H2'    | 48:5:2908:U:O4'    | 2.15                     | 0.47              |
| 49:7:117:G:C2      | 49:7:118:C:C2      | 3.03                     | 0.47              |
| 48:5:2743:A:C2     | 48:5:2744:A:C4     | 3.03                     | 0.47              |
| 50:8:71:A:C2       | 50:8:88:A:H1'      | 2.50                     | 0.47              |
| 51:9:942:G:N2      | 66:OO:138:ASP:OD1  | 2.47                     | 0.47              |
| 48:5:2468:U:N3     | 48:5:2473:A:C6     | 2.83                     | 0.47              |
| 51:9:1267:C:C2     | 51:9:1516:G:C2     | 3.03                     | 0.47              |
| 51:9:1129:G:H3'    | 51:9:1130:G:C8     | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:1240:G:C2     | 48:5:1241:C:C2     | 3.03                     | 0.47              |
| 48:5:2089:G:C6     | 48:5:2262:G:H2'    | 2.50                     | 0.47              |
| 56:EE:160:ILE:HG21 | 56:EE:169:ILE:HG22 | 1.96                     | 0.47              |
| 14:O:160:ARG:NH2   | 48:5:4759:C:OP1    | 2.47                     | 0.47              |
| 63:LL:126:VAL:HG22 | 63:LL:142:VAL:HG13 | 1.97                     | 0.47              |
| 48:5:1886:G:N2     | 48:5:1894:C:C2     | 2.83                     | 0.47              |
| 48:5:100:C:O4'     | 48:5:100:C:O2      | 2.33                     | 0.47              |
| 48:5:1189:G:C2     | 48:5:1190:C:C2     | 3.03                     | 0.47              |
| 7:G:100:HIS:HA     | 7:G:103:ARG:HD2    | 1.95                     | 0.47              |
| 51:9:1141:G:N2     | 51:9:1147:C:C2     | 2.83                     | 0.47              |
| 48:5:4942:C:O3'    | 48:5:4944:C:P      | 2.73                     | 0.47              |
| 48:5:698:G:N2      | 48:5:699:C:C2      | 2.83                     | 0.47              |
| 48:5:1584:G:C6     | 48:5:1585:C:C4     | 3.02                     | 0.47              |
| 51:9:380:G:OP2     | 60:II:181:GLN:NE2  | 2.48                     | 0.47              |
| 8:H:126:VAL:HG11   | 8:H:161:ILE:HG22   | 1.97                     | 0.47              |
| 52:AA:155:ARG:NE   | 73:VV:61:ARG:O     | 2.37                     | 0.47              |
| 5:E:59:TYR:CZ      | 5:E:64:LEU:HB2     | 2.49                     | 0.47              |
| 51:9:830:A:N6      | 51:9:844:U:C4      | 2.72                     | 0.47              |
| 66:OO:126:ILE:HG21 | 66:OO:129:ILE:HD11 | 1.97                     | 0.47              |
| 51:9:102:A:O2'     | 51:9:103:A:OP2     | 2.27                     | 0.47              |
| 1:A:69:PHE:CD1     | 11:L:65:ARG:HD3    | 106.38                   | 0.47              |
| 51:9:1528:G:N1     | 51:9:1529:C:C4     | 2.83                     | 0.47              |
| 48:5:1639:U:H3     | 48:5:1643:A:HO2'   | 1.58                     | 0.47              |
| 51:9:1500:G:H2'    | 51:9:1501:C:O4'    | 2.14                     | 0.47              |
| 48:5:1383:G:C6     | 48:5:1384:C:C4     | 3.02                     | 0.47              |
| 48:5:2743:A:H2'    | 48:5:2744:A:C8     | 2.50                     | 0.47              |
| 14:O:26:GLN:OE1    | 14:O:31:ARG:NH1    | 2.48                     | 0.47              |
| 48:5:2065:G:C6     | 48:5:2066:C:C4     | 3.03                     | 0.47              |
| 48:5:967:C:N3      | 48:5:2254:G:C6     | 2.82                     | 0.47              |
| 4:D:43:LYS:HB3     | 4:D:46:THR:CG2     | 2.45                     | 0.47              |
| 51:9:1335:G:C6     | 51:9:1336:C:C4     | 3.03                     | 0.47              |
| 51:9:1406:G:O3'    | 51:9:1408:U:OP1    | 2.33                     | 0.46              |
| 56:EE:31:PRO:HD2   | 56:EE:38:LEU:HD13  | 1.97                     | 0.46              |
| 51:9:1859:A:H2'    | 51:9:1860:A:C8     | 2.50                     | 0.46              |
| 48:5:1541:C:C2     | 48:5:1619:G:N2     | 2.82                     | 0.46              |
| 56:EE:156:MET:O    | 56:EE:157:ASN:CB   | 2.63                     | 0.46              |
| 51:9:1139:C:O4'    | 51:9:1139:C:O2     | 2.33                     | 0.46              |
| 2:B:240:LEU:HB3    | 2:B:241:PRO:HD2    | 1.96                     | 0.46              |
| 48:5:1995:G:C6     | 48:5:1996:C:C4     | 3.03                     | 0.46              |
| 48:5:2858:A:O2'    | 48:5:2859:G:C8     | 2.65                     | 0.46              |
| 15:P:32:THR:HG21   | 15:P:87:SER:HB3    | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:2771:G:C6    | 48:5:2772:C:C4    | 3.03                     | 0.46              |
| 48:5:1221:G:O2'   | 48:5:1222:A:O5'   | 2.22                     | 0.46              |
| 48:5:1732:C:C2    | 48:5:1798:G:C2    | 3.03                     | 0.46              |
| 49:7:86:G:C2      | 49:7:92:C:C2      | 3.03                     | 0.46              |
| 23:X:52:LEU:HD22  | 23:X:53:ARG:N     | 2.30                     | 0.46              |
| 21:V:38:TYR:N     | 21:V:64:THR:O     | 2.47                     | 0.46              |
| 48:5:1957:U:O2'   | 48:5:1958:A:O4'   | 2.33                     | 0.46              |
| 50:8:56:G:C2      | 50:8:57:C:C2      | 3.03                     | 0.46              |
| 45:1:57:ARG:HH22  | 48:5:3862:A:HO2'  | 1.57                     | 0.46              |
| 48:5:199:G:N1     | 48:5:220:C:C2     | 2.83                     | 0.46              |
| 15:P:41:ILE:HD12  | 15:P:150:LEU:CD1  | 2.46                     | 0.46              |
| 48:5:302:C:N4     | 48:5:303:C:N4     | 2.64                     | 0.46              |
| 51:9:290:U:OP1    | 56:EE:156:MET:HE2 | 2.16                     | 0.46              |
| 48:5:4461:C:C2    | 48:5:4516:G:C2    | 3.03                     | 0.46              |
| 51:9:125:C:OP2    | 58:GG:198:ARG:NH1 | 2.39                     | 0.46              |
| 75:XX:9:THR:O     | 75:XX:11:ARG:N    | 2.48                     | 0.46              |
| 48:5:2245:G:C2    | 48:5:2246:C:C2    | 3.04                     | 0.46              |
| 6:F:98:ARG:HH21   | 6:F:226:THR:HG22  | 1.81                     | 0.46              |
| 20:U:46:ARG:O     | 20:U:47:ILE:C     | 2.53                     | 0.46              |
| 51:9:479:C:H2'    | 51:9:480:G:O4'    | 2.16                     | 0.46              |
| 51:9:562:U:H2'    | 51:9:563:G:C8     | 2.49                     | 0.46              |
| 48:5:4661:G:C6    | 48:5:4662:C:C4    | 3.03                     | 0.46              |
| 48:5:1099:C:H2'   | 48:5:1100:U:O4'   | 2.16                     | 0.46              |
| 48:5:978:G:C6     | 48:5:979:C:C4     | 3.04                     | 0.46              |
| 48:5:106:A:O2'    | 48:5:335:A:N3     | 2.43                     | 0.46              |
| 51:9:1641:A:OP2   | 51:9:1641:A:H8    | 1.99                     | 0.46              |
| 48:5:22:G:N1      | 50:8:35:C:C4      | 2.83                     | 0.46              |
| 13:N:68:ARG:CG    | 48:5:302:C:OP1    | 2.63                     | 0.46              |
| 19:T:64:VAL:HG22  | 19:T:72:VAL:HG11  | 1.97                     | 0.46              |
| 2:B:252:ALA:HB1   | 48:5:4524:G:N3    | 2.30                     | 0.46              |
| 74:WW:52:ILE:HG22 | 74:WW:61:ILE:HG23 | 1.96                     | 0.46              |
| 56:EE:65:CYS:SG   | 56:EE:66:MET:N    | 2.88                     | 0.46              |
| 17:R:119:MET:HG3  | 17:R:123:LEU:HD22 | 1.97                     | 0.46              |
| 48:5:1198:G:H2'   | 48:5:1199:G:C8    | 2.49                     | 0.46              |
| 48:5:4740:G:C2    | 48:5:4741:C:C2    | 3.04                     | 0.46              |
| 51:9:358:C:C2     | 51:9:405:G:C2     | 3.03                     | 0.46              |
| 6:F:41:GLN:CG     | 48:5:2095:A:N1    | 2.79                     | 0.46              |
| 50:8:127:U:C4     | 50:8:128:C:C5     | 3.03                     | 0.46              |
| 48:5:4537:C:H2'   | 48:5:4538:G:C8    | 2.50                     | 0.46              |
| 48:5:1928:C:C4    | 48:5:2054:U:O2    | 2.69                     | 0.46              |
| 48:5:747:A:C2     | 48:5:749:G:HI1'   | 2.50                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:8:55:U:N3      | 50:8:62:A:C2       | 2.83                     | 0.46              |
| 9:I:87:ILE:HG12   | 9:I:138:ILE:CG1    | 2.45                     | 0.46              |
| 51:9:1835:A:N9    | 51:9:1863:A:N7     | 2.63                     | 0.46              |
| 48:5:3766:A:N1    | 51:9:1827:U:O2'    | 2.33                     | 0.46              |
| 56:EE:54:TYR:CD1  | 76:YY:17:LEU:HD11  | 2.51                     | 0.46              |
| 48:5:1984:A:N6    | 48:5:2011:C:O2'    | 2.48                     | 0.46              |
| 48:5:205:C:C4     | 48:5:211:G:C6      | 3.04                     | 0.46              |
| 48:5:384:A:C6     | 48:5:386:A:C5      | 3.04                     | 0.46              |
| 59:HH:145:ARG:HD3 | 74:WW:51:GLU:HB3   | 1.97                     | 0.46              |
| 48:5:1591:U:N3    | 48:5:4555:U:OP1    | 2.47                     | 0.46              |
| 48:5:479:G:N2     | 48:5:480:C:C2      | 2.83                     | 0.46              |
| 63:LL:106:HIS:CG  | 63:LL:106:HIS:O    | 2.69                     | 0.46              |
| 48:5:4587:G:C2    | 48:5:4716:C:C2     | 3.04                     | 0.46              |
| 51:9:23:G:C6      | 51:9:24:C:C4       | 3.03                     | 0.46              |
| 1:A:209:HIS:CG    | 1:A:210:PRO:HD2    | 2.51                     | 0.46              |
| 47:3:35:U:C1'     | 51:9:1641:A:P      | 3.03                     | 0.46              |
| 48:5:4372:U:O2    | 48:5:4377:G:H1'    | 2.15                     | 0.46              |
| 48:5:499:G:C2     | 48:5:500:G:C8      | 3.03                     | 0.46              |
| 48:5:1270:A:H2'   | 48:5:1271:G:O4'    | 2.16                     | 0.46              |
| 51:9:1726:G:C6    | 51:9:1727:G:C5     | 3.03                     | 0.46              |
| 48:5:3900:G:H5''  | 48:5:3901:A:H4'    | 1.97                     | 0.46              |
| 48:5:4916:G:C6    | 48:5:4917:C:C4     | 3.04                     | 0.46              |
| 48:5:1171:G:C6    | 48:5:1172:C:C4     | 3.04                     | 0.46              |
| 48:5:120:A:C2     | 48:5:148:C:O2      | 2.68                     | 0.46              |
| 48:5:2046:G:C2    | 48:5:2047:A:C2     | 3.03                     | 0.46              |
| 48:5:2698:G:C6    | 48:5:2699:C:C4     | 3.03                     | 0.46              |
| 2:B:119:TYR:OH    | 2:B:129:ALA:N      | 2.48                     | 0.46              |
| 48:5:1855:G:C6    | 48:5:1856:C:C4     | 3.04                     | 0.46              |
| 48:5:721:G:C2     | 48:5:948:C:C2      | 3.03                     | 0.46              |
| 51:9:187:G:C6     | 51:9:188:C:C4      | 3.04                     | 0.46              |
| 48:5:4102:C:C2    | 48:5:4108:G:C2     | 3.03                     | 0.46              |
| 56:EE:199:GLU:HB2 | 56:EE:207:VAL:HG12 | 1.97                     | 0.46              |
| 48:5:654:C:H2'    | 48:5:654:C:O2      | 2.15                     | 0.46              |
| 48:5:497:G:H3'    | 48:5:498:C:H5''    | 1.97                     | 0.46              |
| 48:5:1269:G:C8    | 48:5:2111:G:C6     | 3.04                     | 0.46              |
| 48:5:2128:G:C2    | 48:5:2129:C:C2     | 3.03                     | 0.46              |
| 48:5:1643:A:H2'   | 48:5:1644:C:C6     | 2.50                     | 0.46              |
| 48:5:2618:G:C2    | 48:5:2720:C:C2     | 3.03                     | 0.46              |
| 48:5:2698:G:C2    | 48:5:2699:C:C2     | 3.04                     | 0.46              |
| 48:5:1826:G:C6    | 48:5:1827:C:C4     | 3.03                     | 0.46              |
| 71:TT:56:ARG:HD2  | 71:TT:79:TYR:CD2   | 2.50                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:4:ARG:HG3     | 48:5:4458:C:N4     | 2.30                     | 0.46              |
| 51:9:1703:C:O2    | 51:9:1832:A:N1     | 2.48                     | 0.46              |
| 51:9:1096:G:OP1   | 74:WW:22:LYS:NZ    | 2.46                     | 0.46              |
| 51:9:1650:A:C5    | 51:9:1675:A:C2     | 3.03                     | 0.46              |
| 5:E:262:GLN:N     | 48:5:4930:C:OP1    | 2.47                     | 0.46              |
| 48:5:3597:G:C2    | 48:5:3598:C:C2     | 3.03                     | 0.46              |
| 70:SS:66:ARG:HD2  | 70:SS:70:ILE:HD11  | 1.97                     | 0.46              |
| 48:5:177:G:C6     | 48:5:178:C:C4      | 3.03                     | 0.46              |
| 74:WW:105:THR:HB  | 74:WW:126:LEU:HD11 | 1.97                     | 0.46              |
| 48:5:1279:A:C4    | 48:5:1280:C:C4     | 3.04                     | 0.46              |
| 48:5:1280:C:N3    | 48:5:1282:G:C6     | 2.83                     | 0.46              |
| 48:5:1379:C:H4'   | 48:5:1380:G:C8     | 2.50                     | 0.46              |
| 51:9:993:G:C2     | 51:9:994:C:C2      | 3.04                     | 0.46              |
| 51:9:752:G:N1     | 51:9:790:C:C4      | 2.83                     | 0.46              |
| 48:5:4919:G:C6    | 48:5:4920:C:C4     | 3.04                     | 0.46              |
| 51:9:1401:A:H2'   | 51:9:1402:A:C8     | 2.51                     | 0.46              |
| 48:5:1365:C:O2    | 48:5:1366:G:C8     | 2.69                     | 0.46              |
| 74:WW:53:ILE:HD11 | 74:WW:62:VAL:HG23  | 1.98                     | 0.46              |
| 48:5:177:G:C2     | 48:5:178:C:C2      | 3.03                     | 0.46              |
| 69:RR:36:GLU:HG2  | 69:RR:47:ARG:HD2   | 1.98                     | 0.46              |
| 48:5:2818:C:OP1   | 48:5:4655:A:H4'    | 2.15                     | 0.46              |
| 18:S:83:ARG:HH21  | 18:S:83:ARG:CG     | 2.29                     | 0.46              |
| 52:AA:159:ILE:O   | 52:AA:159:ILE:HG23 | 2.16                     | 0.46              |
| 46:2:30:G:C6      | 46:2:31:C:C4       | 3.04                     | 0.46              |
| 48:5:207:G:O4'    | 48:5:406:C:H5'     | 2.15                     | 0.46              |
| 74:WW:26:LEU:HD11 | 74:WW:60:LYS:HD3   | 1.96                     | 0.46              |
| 51:9:872:A:N6     | 51:9:914:U:C4      | 2.83                     | 0.46              |
| 48:5:4283:G:N1    | 48:5:4284:C:C4     | 2.84                     | 0.46              |
| 2:B:156:TYR:CD1   | 48:5:4909:A:C2'    | 2.91                     | 0.46              |
| 48:5:917:A:C6     | 48:5:919:C:N4      | 2.84                     | 0.46              |
| 48:5:746:A:H4'    | 48:5:747:A:OP1     | 2.16                     | 0.46              |
| 51:9:1454:A:P     | 69:RR:3:ARG:HE     | 2.39                     | 0.46              |
| 48:5:1240:G:C6    | 48:5:1241:C:C4     | 3.04                     | 0.46              |
| 48:5:199:G:C2     | 48:5:201:C:N3      | 2.84                     | 0.46              |
| 51:9:834:C:N4     | 51:9:841:G:C6      | 2.84                     | 0.46              |
| 56:EE:126:VAL:CG1 | 56:EE:160:ILE:HD11 | 2.46                     | 0.46              |
| 48:5:3586:G:C2    | 48:5:3587:C:C2     | 3.03                     | 0.46              |
| 48:5:967:C:OP1    | 48:5:2254:G:N1     | 2.48                     | 0.46              |
| 1:A:112:ILE:HG23  | 1:A:133:TYR:CD2    | 2.51                     | 0.46              |
| 48:5:2847:G:N2    | 48:5:3842:C:C2     | 2.84                     | 0.46              |
| 5:E:41:SER:HA     | 48:5:978:G:H4'     | 1.96                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:3:38:A:C2      | 57:FF:135:ARG:CZ   | 2.98                     | 0.46              |
| 47:3:38:A:N3      | 57:FF:135:ARG:NH2  | 2.63                     | 0.46              |
| 51:9:1466:G:C6    | 51:9:1467:C:N4     | 2.84                     | 0.46              |
| 48:5:3900:G:C2    | 48:5:4562:C:N3     | 2.84                     | 0.46              |
| 74:WW:27:ILE:HG12 | 74:WW:61:ILE:HB    | 1.97                     | 0.46              |
| 2:B:29:VAL:CG2    | 2:B:346:THR:HG21   | 2.46                     | 0.46              |
| 47:3:24:G:H2'     | 47:3:25:C:O4'      | 2.16                     | 0.46              |
| 47:3:24:G:C2      | 47:3:25:C:C2       | 3.03                     | 0.46              |
| 14:O:12:ARG:O     | 18:S:171:ARG:NH2   | 2.49                     | 0.46              |
| 48:5:3600:G:C6    | 48:5:3601:C:C4     | 3.04                     | 0.46              |
| 67:PP:53:GLN:HE22 | 67:PP:83:MET:HG3   | 1.80                     | 0.46              |
| 48:5:4472:G:C6    | 48:5:4473:A:N7     | 2.84                     | 0.46              |
| 58:GG:66:GLY:O    | 58:GG:68:LEU:HD22  | 2.16                     | 0.46              |
| 48:5:1416:G:N2    | 48:5:1417:C:C2     | 2.84                     | 0.46              |
| 57:FF:99:ILE:HD11 | 77:ZZ:106:GLN:HE22 | 1.81                     | 0.46              |
| 5:E:250:ASP:O     | 5:E:254:LEU:N      | 2.46                     | 0.46              |
| 48:5:918:G:H2'    | 48:5:918:G:N3      | 2.31                     | 0.46              |
| 48:5:3729:U:H2'   | 48:5:3730:U:C6     | 2.52                     | 0.46              |
| 51:9:1102:G:C2    | 51:9:1103:C:C4     | 3.04                     | 0.46              |
| 1:A:19:HIS:NE2    | 48:5:1338:G:N2     | 68.37                    | 0.46              |
| 48:5:3717:A:O2'   | 48:5:3718:A:O4'    | 2.33                     | 0.46              |
| 48:5:1613:A:H3'   | 48:5:1614:C:C5'    | 2.46                     | 0.46              |
| 48:5:705:G:N2     | 48:5:706:C:C2      | 2.84                     | 0.46              |
| 48:5:4136:G:C2    | 48:5:4137:C:C2     | 3.04                     | 0.46              |
| 48:5:2065:G:H2'   | 48:5:2066:C:O4'    | 2.16                     | 0.46              |
| 48:5:2065:G:C2    | 48:5:2066:C:C2     | 3.04                     | 0.46              |
| 6:F:41:GLN:HG3    | 48:5:2095:A:N1     | 2.31                     | 0.46              |
| 51:9:1319:U:H2'   | 51:9:1320:G:O4'    | 2.16                     | 0.46              |
| 48:5:4737:G:C2    | 48:5:4738:C:C2     | 3.04                     | 0.46              |
| 13:N:169:ARG:NH1  | 48:5:63:G:OP2      | 2.43                     | 0.46              |
| 46:2:54:U:H2'     | 46:2:55:U:O4'      | 2.16                     | 0.46              |
| 51:9:1563:G:C2    | 51:9:1564:C:C2     | 3.04                     | 0.46              |
| 12:M:37:LEU:HD23  | 18:S:100:LEU:HD11  | 1.98                     | 0.46              |
| 48:5:726:G:C6     | 48:5:727:C:N4      | 2.84                     | 0.46              |
| 48:5:181:C:C4     | 48:5:256:G:N1      | 2.84                     | 0.45              |
| 75:XX:57:VAL:HG11 | 75:XX:115:ILE:HG22 | 1.97                     | 0.45              |
| 1:A:207:VAL:HG12  | 48:5:3919:C:H4'    | 1.97                     | 0.45              |
| 48:5:1639:U:H2'   | 48:5:1639:U:O2     | 2.16                     | 0.45              |
| 48:5:2711:G:H3'   | 48:5:2712:G:H5''   | 1.98                     | 0.45              |
| 48:5:984:C:C2     | 48:5:1070:G:N2     | 2.84                     | 0.45              |
| 48:5:5017:G:C2    | 48:5:5018:C:C2     | 3.05                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:5:5017:G:C6     | 48:5:5018:C:C4    | 3.04                     | 0.45              |
| 7:G:221:ALA:O      | 7:G:224:THR:OG1   | 2.34                     | 0.45              |
| 48:5:2270:G:C6     | 48:5:2271:C:C4    | 3.04                     | 0.45              |
| 48:5:3941:G:H2'    | 48:5:3942:A:O4'   | 2.15                     | 0.45              |
| 7:G:58:PRO:HD3     | 23:X:46:PHE:HD2   | 1.80                     | 0.45              |
| 48:5:3690:U:H2'    | 48:5:3691:G:O4'   | 2.17                     | 0.45              |
| 48:5:2569:G:H2'    | 48:5:2570:U:O4'   | 2.15                     | 0.45              |
| 54:CC:192:LEU:HD23 | 54:CC:227:TRP:HE1 | 1.77                     | 0.45              |
| 47:3:29:A:HO2'     | 47:3:30:G:P       | 2.33                     | 0.45              |
| 51:9:305:U:O2'     | 51:9:309:G:O4'    | 2.28                     | 0.45              |
| 60:II:55:TYR:HB2   | 60:II:182:CYS:O   | 2.16                     | 0.45              |
| 51:9:1862:G:N2     | 51:9:1863:A:H2    | 2.13                     | 0.45              |
| 48:5:3942:A:H2'    | 48:5:3943:A:O4'   | 2.17                     | 0.45              |
| 48:5:4904:G:N2     | 48:5:4905:C:C2    | 2.85                     | 0.45              |
| 73:VV:30:ALA:O     | 73:VV:60:ARG:HD3  | 2.17                     | 0.45              |
| 48:5:4881:U:O2     | 48:5:4881:U:O4'   | 2.34                     | 0.45              |
| 48:5:4423:U:O2     | 48:5:4423:U:O4'   | 2.34                     | 0.45              |
| 51:9:997:A:H2'     | 51:9:998:A:O4'    | 2.16                     | 0.45              |
| 48:5:4773:C:C2     | 48:5:4863:G:C2    | 3.04                     | 0.45              |
| 46:2:7:G:C6        | 46:2:49:C:N4      | 2.84                     | 0.45              |
| 48:5:35:U:O2'      | 48:5:1525:A:N1    | 2.46                     | 0.45              |
| 47:3:67:U:C2'      | 47:3:68:C:C5'     | 2.77                     | 0.45              |
| 48:5:77:U:H3       | 48:5:336:A:N6     | 2.13                     | 0.45              |
| 51:9:434:G:N3      | 51:9:473:A:H2     | 2.13                     | 0.45              |
| 12:M:119:ARG:NH2   | 14:O:189:ILE:HD12 | 2.31                     | 0.45              |
| 48:5:4883:C:O2'    | 48:5:4884:G:P     | 2.74                     | 0.45              |
| 48:5:1904:G:N2     | 48:5:2073:C:C2    | 2.84                     | 0.45              |
| 48:5:688:U:H2'     | 48:5:689:U:C6     | 2.52                     | 0.45              |
| 51:9:23:G:C2       | 51:9:24:C:C2      | 3.04                     | 0.45              |
| 48:5:1826:G:C2     | 48:5:1827:C:C2    | 3.04                     | 0.45              |
| 4:D:111:ASN:ND2    | 4:D:111:ASN:C     | 2.70                     | 0.45              |
| 51:9:591:U:O4'     | 51:9:591:U:O2     | 2.31                     | 0.45              |
| 48:5:2465:C:H2'    | 48:5:2466:G:C8    | 2.51                     | 0.45              |
| 24:Y:59:ARG:NH2    | 48:5:200:U:O2'    | 2.49                     | 0.45              |
| 63:LL:35:ARG:NH2   | 63:LL:55:TYR:O    | 2.43                     | 0.45              |
| 48:5:4699:U:C4     | 48:5:4702:G:C6    | 3.05                     | 0.45              |
| 48:5:5001:U:H2'    | 48:5:5002:U:O4'   | 2.16                     | 0.45              |
| 51:9:1673:U:H2'    | 51:9:1674:G:O4'   | 2.16                     | 0.45              |
| 51:9:673:G:C6      | 51:9:674:C:C4     | 3.04                     | 0.45              |
| 51:9:1409:A:C6     | 51:9:1410:C:C5    | 3.04                     | 0.45              |
| 48:5:504:G:O6      | 48:5:654:C:C4     | 2.70                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:Q:14:ARG:NH2   | 48:5:2083:C:OP2    | 2.49                     | 0.45              |
| 48:5:4109:G:C6    | 48:5:4110:C:C4     | 3.05                     | 0.45              |
| 48:5:1098:G:C2    | 48:5:1099:C:C2     | 3.05                     | 0.45              |
| 73:VV:32:ILE:HD12 | 73:VV:60:ARG:HD2   | 1.97                     | 0.45              |
| 63:LL:76:VAL:HB   | 63:LL:125:ILE:HD13 | 1.98                     | 0.45              |
| 48:5:4644:G:C6    | 48:5:4645:C:C4     | 3.05                     | 0.45              |
| 73:VV:47:ASN:O    | 73:VV:49:GLN:N     | 2.49                     | 0.45              |
| 77:ZZ:58:LEU:HD23 | 77:ZZ:62:VAL:HG21  | 1.97                     | 0.45              |
| 48:5:190:G:C2     | 48:5:252:C:C2      | 3.04                     | 0.45              |
| 51:9:1294:G:C6    | 51:9:1295:A:C5     | 3.04                     | 0.45              |
| 51:9:1298:G:O2'   | 51:9:1299:A:C8     | 2.69                     | 0.45              |
| 53:BB:33:VAL:HG21 | 53:BB:67:PHE:CZ    | 2.52                     | 0.45              |
| 48:5:977:C:O2'    | 48:5:978:G:H5'     | 2.17                     | 0.45              |
| 5:E:124:HIS:NE2   | 48:5:1282:G:N7     | 2.65                     | 0.45              |
| 51:9:293:C:O2'    | 51:9:294:U:H3'     | 2.16                     | 0.45              |
| 48:5:2395:A:HO2'  | 48:5:2806:A:H1'    | 1.77                     | 0.45              |
| 47:3:35:U:O4'     | 51:9:1641:A:P      | 2.74                     | 0.45              |
| 51:9:1489:A:H4'   | 51:9:1490:G:OP2    | 2.15                     | 0.45              |
| 48:5:3918:G:C6    | 48:5:3919:C:C4     | 3.04                     | 0.45              |
| 48:5:1549:G:N2    | 48:5:1580:C:C2     | 2.84                     | 0.45              |
| 48:5:1995:G:C6    | 48:5:1996:C:N3     | 2.84                     | 0.45              |
| 48:5:1925:G:C6    | 48:5:1926:C:C4     | 3.05                     | 0.45              |
| 14:O:116:LYS:HD3  | 18:S:169:THR:HG21  | 1.98                     | 0.45              |
| 51:9:194:C:C2     | 51:9:206:G:C2      | 3.05                     | 0.45              |
| 9:I:93:PRO:HB2    | 9:I:125:THR:HB     | 1.99                     | 0.45              |
| 48:5:2567:G:C2    | 48:5:2568:C:C2     | 3.04                     | 0.45              |
| 60:II:139:LYS:HD2 | 60:II:145:ILE:HD12 | 1.99                     | 0.45              |
| 48:5:5008:C:H2'   | 48:5:5009:G:O4'    | 2.16                     | 0.45              |
| 15:P:41:ILE:HD12  | 15:P:150:LEU:HD13  | 1.99                     | 0.45              |
| 48:5:1448:G:C2    | 48:5:1449:C:C2     | 3.04                     | 0.45              |
| 51:9:1537:A:N1    | 51:9:1596:U:O4     | 2.50                     | 0.45              |
| 48:5:1072:C:O2    | 48:5:1072:C:H2'    | 2.17                     | 0.45              |
| 13:N:179:LYS:O    | 48:5:298:G:H5'     | 2.16                     | 0.45              |
| 48:5:4473:A:H2'   | 48:5:4474:A:C8     | 2.51                     | 0.45              |
| 51:9:1274:G:N7    | 62:KK:43:LEU:HD13  | 2.32                     | 0.45              |
| 72:UU:46:LYS:HD3  | 72:UU:97:ILE:HG23  | 1.98                     | 0.45              |
| 74:WW:8:ALA:HA    | 74:WW:74:VAL:HG11  | 1.97                     | 0.45              |
| 48:5:3727:A:H2'   | 48:5:3728:A:C8     | 2.51                     | 0.45              |
| 57:FF:143:PRO:O   | 57:FF:147:VAL:HG23 | 2.16                     | 0.45              |
| 48:5:199:G:C6     | 48:5:220:C:N3      | 2.85                     | 0.45              |
| 48:5:351:C:C2     | 50:8:25:G:C2       | 3.04                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:5020:G:C6    | 48:5:5021:C:C4     | 3.04                     | 0.45              |
| 51:9:1541:G:C2    | 51:9:1542:C:C2     | 3.05                     | 0.45              |
| 48:5:2664:G:N2    | 48:5:2671:C:C2     | 2.85                     | 0.45              |
| 51:9:1597:C:H4'   | 51:9:1603:G:C6     | 2.52                     | 0.45              |
| 74:WW:82:GLN:O    | 74:WW:84:LYS:N     | 2.49                     | 0.45              |
| 49:7:27:G:C2      | 49:7:28:C:C2       | 3.05                     | 0.45              |
| 48:5:488:G:N2     | 48:5:489:C:C2      | 2.85                     | 0.45              |
| 70:SS:113:ARG:HG2 | 70:SS:113:ARG:HH11 | 1.81                     | 0.45              |
| 72:UU:68:THR:HG22 | 72:UU:69:PRO:O     | 2.17                     | 0.45              |
| 51:9:1041:G:C2    | 51:9:1075:C:C2     | 3.04                     | 0.45              |
| 59:HH:177:TYR:CZ  | 59:HH:181:THR:HG21 | 2.51                     | 0.45              |
| 61:JJ:94:LEU:HD12 | 61:JJ:97:ILE:HD12  | 1.98                     | 0.45              |
| 48:5:179:G:C2     | 48:5:180:C:C2      | 3.05                     | 0.45              |
| 16:Q:17:GLU:HB2   | 16:Q:18:PRO:HD2    | 1.98                     | 0.45              |
| 48:5:1322:A:N6    | 48:5:4446:U:OP1    | 2.48                     | 0.45              |
| 9:I:49:CYS:HG     | 9:I:51:HIS:CD2     | 2.32                     | 0.45              |
| 51:9:1267:C:HO2'  | 51:9:1268:C:H5'    | 1.77                     | 0.45              |
| 48:5:1241:C:C2'   | 48:5:1242:G:OP1    | 2.65                     | 0.45              |
| 71:TT:62:ARG:C    | 71:TT:62:ARG:HD2   | 2.37                     | 0.45              |
| 48:5:2594:C:C2    | 48:5:2752:G:C2     | 3.04                     | 0.45              |
| 48:5:1855:G:C2    | 48:5:1856:C:C2     | 3.04                     | 0.45              |
| 51:9:1294:G:O2'   | 51:9:1295:A:O5'    | 2.29                     | 0.45              |
| 50:8:94:G:H5'     | 50:8:94:G:C8       | 2.52                     | 0.45              |
| 64:MM:50:CYS:SG   | 64:MM:51:VAL:N     | 2.90                     | 0.45              |
| 51:9:1717:C:C2    | 51:9:1817:G:C2     | 3.04                     | 0.45              |
| 51:9:1749:G:C2    | 51:9:1750:C:C2     | 3.05                     | 0.45              |
| 48:5:994:G:C2     | 48:5:1050:C:C2     | 3.04                     | 0.45              |
| 66:OO:62:VAL:HG21 | 66:OO:73:ALA:HB2   | 1.98                     | 0.45              |
| 59:HH:115:LYS:O   | 59:HH:116:ARG:CB   | 2.65                     | 0.45              |
| 48:5:1959:U:H1'   | 48:5:1961:G:O4'    | 2.17                     | 0.45              |
| 9:I:202:ASN:N     | 9:I:202:ASN:OD1    | 2.49                     | 0.45              |
| 5:E:157:ARG:HD3   | 5:E:266:TYR:CZ     | 2.52                     | 0.45              |
| 58:GG:173:ALA:HB1 | 58:GG:174:PRO:CD   | 2.47                     | 0.45              |
| 51:9:751:G:O2'    | 51:9:752:G:O4'     | 2.25                     | 0.45              |
| 48:5:1744:U:H2'   | 48:5:1745:G:O4'    | 2.17                     | 0.45              |
| 25:Z:55:ALA:O     | 25:Z:57:MET:N      | 2.49                     | 0.45              |
| 48:5:4473:A:C2    | 48:5:4474:A:C5     | 3.04                     | 0.45              |
| 48:5:994:G:C2     | 48:5:995:C:C2      | 3.05                     | 0.45              |
| 51:9:797:C:O2     | 51:9:798:G:O2'     | 2.35                     | 0.45              |
| 48:5:2898:G:C6    | 48:5:2899:C:C4     | 3.05                     | 0.45              |
| 66:OO:65:ASP:OD1  | 66:OO:65:ASP:N     | 2.50                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:5:4874:A:H3'    | 48:5:4875:G:C5'   | 2.47                     | 0.45              |
| 58:GG:76:LEU:HD22  | 58:GG:92:ARG:CG   | 2.47                     | 0.45              |
| 48:5:158:A:H5''    | 48:5:159:C:H2'    | 1.99                     | 0.45              |
| 51:9:1759:G:C2     | 51:9:1774:C:C2    | 3.05                     | 0.45              |
| 59:HH:15:LYS:N     | 59:HH:16:PRO:HD2  | 2.32                     | 0.45              |
| 60:II:25:ARG:O     | 60:II:27:TYR:N    | 2.50                     | 0.45              |
| 48:5:4207:C:C2     | 48:5:4226:G:N2    | 2.85                     | 0.45              |
| 48:5:1070:G:C6     | 48:5:1071:C:N4    | 2.85                     | 0.45              |
| 14:O:85:ARG:NH2    | 48:5:3887:C:OP2   | 2.43                     | 0.45              |
| 48:5:2245:G:C6     | 48:5:2246:C:C4    | 3.05                     | 0.45              |
| 51:9:1563:G:C6     | 51:9:1564:C:C4    | 3.05                     | 0.45              |
| 51:9:673:G:C2      | 51:9:674:C:C2     | 3.05                     | 0.45              |
| 48:5:994:G:C6      | 48:5:995:C:C4     | 3.05                     | 0.45              |
| 51:9:1218:C:H6     | 51:9:1218:C:O5'   | 2.00                     | 0.45              |
| 48:5:4183:G:N3     | 48:5:4183:G:H2'   | 2.32                     | 0.45              |
| 48:5:202:C:C2      | 48:5:214:G:C2     | 3.04                     | 0.45              |
| 48:5:751:G:N2      | 48:5:912:G:C4     | 2.84                     | 0.45              |
| 18:S:47:PHE:HE1    | 18:S:125:GLN:HG2  | 1.81                     | 0.45              |
| 48:5:2322:G:C6     | 48:5:2323:C:C4    | 3.05                     | 0.45              |
| 48:5:1947:U:H2'    | 48:5:1947:U:O2    | 2.17                     | 0.45              |
| 23:X:127:LEU:HD12  | 23:X:127:LEU:C    | 2.38                     | 0.45              |
| 54:CC:112:VAL:HG22 | 54:CC:123:ARG:O   | 2.16                     | 0.45              |
| 1:A:233:ARG:O      | 1:A:235:VAL:HB    | 2.17                     | 0.45              |
| 2:B:249:ARG:NH2    | 48:5:3845:A:OP2   | 2.49                     | 0.45              |
| 17:R:4:LEU:HD22    | 17:R:32:ILE:HG22  | 2.00                     | 0.44              |
| 51:9:323:C:H3'     | 51:9:324:C:C5'    | 2.47                     | 0.44              |
| 7:G:159:HIS:CE1    | 7:G:185:LYS:HE2   | 2.51                     | 0.44              |
| 47:3:70:G:O2'      | 47:3:71:G:O4'     | 2.22                     | 0.44              |
| 48:5:973:G:N2      | 48:5:974:C:C2     | 2.85                     | 0.44              |
| 48:5:1404:G:C6     | 48:5:1405:C:C4    | 3.04                     | 0.44              |
| 51:9:832:G:N2      | 51:9:843:C:C2     | 2.85                     | 0.44              |
| 1:A:90:CYS:CB      | 1:A:101:VAL:HG13  | 2.47                     | 0.44              |
| 48:5:4731:G:H4'    | 48:5:4732:G:H5'   | 1.99                     | 0.44              |
| 48:5:2122:G:O2'    | 48:5:2123:C:P     | 2.74                     | 0.44              |
| 48:5:2517:A:N3     | 48:5:2539:C:O2'   | 2.43                     | 0.44              |
| 52:AA:110:ASN:O    | 52:AA:116:PHE:CD1 | 2.71                     | 0.44              |
| 48:5:278:G:H4'     | 48:5:279:A:OP2    | 2.17                     | 0.44              |
| 48:5:1196:G:C6     | 48:5:1197:C:C4    | 3.05                     | 0.44              |
| 59:HH:76:GLN:HE22  | 59:HH:94:PHE:HB2  | 1.82                     | 0.44              |
| 48:5:2313:A:O2'    | 48:5:2314:G:OP1   | 2.22                     | 0.44              |
| 48:5:2715:G:C2     | 48:5:2716:C:C2    | 3.05                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 49:7:111:C:H2'   | 49:7:112:U:O4'    | 2.18                     | 0.44              |
| 51:9:828:G:C6    | 51:9:829:C:C4     | 3.05                     | 0.44              |
| 48:5:2559:G:C6   | 48:5:2560:C:C4    | 3.04                     | 0.44              |
| 14:O:27:VAL:CG1  | 14:O:98:ALA:HB1   | 2.47                     | 0.44              |
| 50:8:134:G:C6    | 50:8:135:C:C4     | 3.05                     | 0.44              |
| 48:5:978:G:C2    | 48:5:979:C:C2     | 3.05                     | 0.44              |
| 48:5:1277:G:N1   | 48:5:1278:C:C4    | 2.85                     | 0.44              |
| 48:5:1268:G:C4   | 48:5:2111:G:N2    | 2.86                     | 0.44              |
| 48:5:1823:G:C3'  | 48:5:1825:A:P     | 3.05                     | 0.44              |
| 48:5:1840:G:C3'  | 48:5:1842:G:P     | 3.05                     | 0.44              |
| 19:T:80:VAL:O    | 19:T:82:GLY:N     | 2.51                     | 0.44              |
| 48:5:4109:G:C2   | 48:5:4110:C:C2    | 3.06                     | 0.44              |
| 48:5:3782:C:C2   | 48:5:3811:G:C2    | 3.05                     | 0.44              |
| 48:5:2594:C:O2   | 48:5:2752:G:C2    | 2.71                     | 0.44              |
| 4:D:146:LEU:HD11 | 4:D:159:VAL:CG1   | 2.47                     | 0.44              |
| 48:5:4740:G:C6   | 48:5:4741:C:C4    | 3.04                     | 0.44              |
| 48:5:1196:G:C2   | 48:5:1197:C:C2    | 3.05                     | 0.44              |
| 48:5:2715:G:C6   | 48:5:2716:C:C4    | 3.05                     | 0.44              |
| 48:5:2682:G:N2   | 48:5:2683:C:C2    | 2.85                     | 0.44              |
| 51:9:697:G:C2    | 51:9:734:C:C2     | 3.04                     | 0.44              |
| 48:5:2315:G:C2   | 48:5:2325:C:C2    | 3.05                     | 0.44              |
| 51:9:508:A:H3'   | 51:9:509:G:H8     | 1.82                     | 0.44              |
| 22:W:44:ARG:HH11 | 22:W:44:ARG:HG2   | 1.81                     | 0.44              |
| 51:9:1612:G:C2   | 51:9:1628:C:C2    | 3.05                     | 0.44              |
| 48:5:2376:A:H2'  | 48:5:2377:C:O4'   | 2.17                     | 0.44              |
| 70:SS:8:LYS:HD3  | 77:ZZ:49:LEU:HD11 | 2.00                     | 0.44              |
| 51:9:1386:A:H2'  | 51:9:1387:G:H8    | 1.82                     | 0.44              |
| 51:9:200:G:C2    | 51:9:201:C:C4     | 3.05                     | 0.44              |
| 51:9:834:C:N3    | 51:9:841:G:N2     | 2.66                     | 0.44              |
| 51:9:1559:C:C2   | 51:9:1577:G:C2    | 3.06                     | 0.44              |
| 48:5:2609:G:C2   | 48:5:2731:C:O2    | 2.70                     | 0.44              |
| 48:5:2909:C:O2   | 48:5:3586:G:C2    | 2.71                     | 0.44              |
| 48:5:1995:G:C5   | 48:5:1996:C:C4    | 3.05                     | 0.44              |
| 49:7:117:G:C6    | 49:7:118:C:C4     | 3.05                     | 0.44              |
| 48:5:751:G:C2    | 48:5:752:G:N7     | 2.84                     | 0.44              |
| 48:5:4451:G:C6   | 48:5:4522:G:C8    | 3.05                     | 0.44              |
| 48:5:4090:G:N2   | 48:5:4160:C:C2    | 2.86                     | 0.44              |
| 2:B:100:ARG:NH1  | 48:5:4911:A:OP2   | 2.50                     | 0.44              |
| 49:7:25:G:C6     | 49:7:26:C:C4      | 3.06                     | 0.44              |
| 48:5:4749:C:O2   | 48:5:4749:C:O4'   | 2.32                     | 0.44              |
| 76:YY:7:ILE:HD11 | 76:YY:40:ILE:HG13 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:9:917:U:H2'    | 51:9:918:U:O4'    | 2.17                     | 0.44              |
| 57:FF:154:LEU:HA  | 57:FF:189:ALA:HB2 | 2.00                     | 0.44              |
| 51:9:594:A:C6     | 51:9:643:A:C8     | 3.06                     | 0.44              |
| 48:5:723:A:C2     | 48:5:724:C:C6     | 3.06                     | 0.44              |
| 51:9:1835:A:C8    | 51:9:1863:A:C8    | 3.06                     | 0.44              |
| 48:5:1296:G:C1'   | 48:5:1297:U:P     | 3.06                     | 0.44              |
| 51:9:841:G:C6     | 51:9:842:C:C4     | 3.05                     | 0.44              |
| 51:9:1552:G:C8    | 51:9:1578:U:C4    | 3.05                     | 0.44              |
| 6:F:146:TYR:CE2   | 6:F:239:GLU:CB    | 3.01                     | 0.44              |
| 48:5:4416:G:N1    | 48:5:4417:C:C4    | 2.86                     | 0.44              |
| 48:5:43:U:C2'     | 48:5:44:A:O5'     | 2.66                     | 0.44              |
| 48:5:52:G:N1      | 48:5:53:C:C4      | 2.86                     | 0.44              |
| 56:EE:15:PRO:HG2  | 56:EE:18:TRP:CZ2  | 2.52                     | 0.44              |
| 51:9:1227:G:C2    | 51:9:1228:A:C8    | 3.06                     | 0.44              |
| 48:5:4088:C:H2'   | 48:5:4089:G:C8    | 2.53                     | 0.44              |
| 48:5:192:G:C2     | 48:5:250:C:C2     | 3.05                     | 0.44              |
| 5:E:169:LEU:HD21  | 5:E:187:GLN:HG3   | 1.98                     | 0.44              |
| 54:CC:196:ILE:HB  | 54:CC:223:TYR:HB2 | 1.99                     | 0.44              |
| 8:H:55:LEU:HD22   | 8:H:77:VAL:HG11   | 2.00                     | 0.44              |
| 75:XX:51:VAL:HG13 | 75:XX:70:VAL:HG13 | 1.99                     | 0.44              |
| 51:9:1573:G:C6    | 51:9:1574:C:N3    | 2.86                     | 0.44              |
| 47:3:5:G:N2       | 47:3:68:C:C2      | 2.85                     | 0.44              |
| 51:9:666:U:C2     | 51:9:667:U:C5     | 3.05                     | 0.44              |
| 47:3:35:U:O2'     | 47:3:36:U:H5'     | 2.17                     | 0.44              |
| 51:9:1446:A:O2'   | 51:9:1447:G:H5''  | 2.18                     | 0.44              |
| 51:9:1839:U:H2'   | 51:9:1840:U:C6    | 2.52                     | 0.44              |
| 48:5:4754:G:N2    | 48:5:4880:C:C2    | 2.86                     | 0.44              |
| 25:Z:29:ILE:HD12  | 25:Z:29:ILE:N     | 2.32                     | 0.44              |
| 51:9:1754:G:C2    | 51:9:1755:C:C2    | 3.05                     | 0.44              |
| 51:9:480:G:C6     | 51:9:481:C:N3     | 2.86                     | 0.44              |
| 48:5:3600:G:C2    | 48:5:3601:C:C2    | 3.06                     | 0.44              |
| 64:MM:35:ILE:HD13 | 64:MM:61:TYR:CE1  | 2.53                     | 0.44              |
| 48:5:5038:A:H2'   | 48:5:5039:U:O4'   | 2.18                     | 0.44              |
| 48:5:4091:G:N2    | 48:5:4159:C:C2    | 2.85                     | 0.44              |
| 51:9:374:G:C2     | 51:9:391:C:C2     | 3.06                     | 0.44              |
| 66:OO:133:THR:O   | 66:OO:135:ILE:N   | 2.49                     | 0.44              |
| 7:G:51:LEU:HD11   | 48:5:4086:G:C4    | 2.53                     | 0.44              |
| 12:M:116:LYS:HE3  | 14:O:201:PHE:CE2  | 2.53                     | 0.44              |
| 48:5:1928:C:N4    | 48:5:2054:U:O2    | 2.51                     | 0.44              |
| 51:9:31:U:O2'     | 51:9:595:U:H4'    | 2.17                     | 0.44              |
| 48:5:2288:G:C2    | 48:5:2290:C:C4    | 3.05                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:3900:G:C2    | 48:5:4562:C:C2     | 3.06                     | 0.44              |
| 48:5:2481:G:C6    | 48:5:2482:C:C4     | 3.05                     | 0.44              |
| 48:5:1430:C:O2    | 48:5:1455:G:C2     | 2.70                     | 0.44              |
| 48:5:1171:G:C2    | 48:5:1172:C:C2     | 3.05                     | 0.44              |
| 48:5:4129:G:C6    | 48:5:4130:C:C4     | 3.05                     | 0.44              |
| 48:5:2315:G:C2    | 48:5:2325:C:O2     | 2.71                     | 0.44              |
| 48:5:3882:C:H2'   | 48:5:3883:U:C6     | 2.53                     | 0.44              |
| 51:9:126:G:N2     | 51:9:180:G:O2'     | 2.49                     | 0.44              |
| 9:I:47:PRO:HB3    | 9:I:171:TRP:CE2    | 2.53                     | 0.44              |
| 75:XX:109:GLY:O   | 75:XX:110:HIS:C    | 2.56                     | 0.44              |
| 50:8:10:G:C2      | 50:8:11:C:C2       | 3.06                     | 0.44              |
| 48:5:1691:G:C6    | 48:5:1692:C:C4     | 3.06                     | 0.44              |
| 51:9:640:A:H2'    | 51:9:641:A:C8      | 2.52                     | 0.44              |
| 54:CC:133:TYR:CD1 | 54:CC:216:MET:HA   | 2.53                     | 0.44              |
| 51:9:1669:G:C6    | 51:9:1670:C:C4     | 3.06                     | 0.44              |
| 48:5:1958:A:C4'   | 48:5:1962:A:O2'    | 2.63                     | 0.44              |
| 14:O:133:ARG:CZ   | 48:5:1928:C:C4     | 3.00                     | 0.44              |
| 48:5:744:G:H2'    | 48:5:745:G:C8      | 2.53                     | 0.44              |
| 51:9:993:G:C6     | 51:9:994:C:C4      | 3.06                     | 0.44              |
| 51:9:103:A:C6     | 51:9:356:C:C2      | 3.06                     | 0.44              |
| 48:5:5016:A:N6    | 48:5:5033:G:O2'    | 2.50                     | 0.44              |
| 48:5:3670:C:O2'   | 48:5:3671:G:O4'    | 2.36                     | 0.44              |
| 48:5:1064:G:C2    | 48:5:1065:G:C4     | 3.06                     | 0.44              |
| 48:5:125:C:C2     | 48:5:145:G:C2      | 3.06                     | 0.44              |
| 51:9:1298:G:O2'   | 51:9:1299:A:O4'    | 2.36                     | 0.44              |
| 48:5:2021:G:C2    | 48:5:2022:C:C2     | 3.06                     | 0.44              |
| 58:GG:7:PHE:CD2   | 58:GG:10:THR:HG23  | 2.53                     | 0.44              |
| 25:Z:54:THR:O     | 25:Z:56:ALA:N      | 2.51                     | 0.44              |
| 63:LL:68:ILE:HG21 | 63:LL:143:LEU:HD21 | 1.99                     | 0.44              |
| 48:5:2275:G:H5''  | 48:5:2275:G:H8     | 1.82                     | 0.44              |
| 51:9:1161:U:O4    | 75:XX:2:GLY:N      | 2.50                     | 0.44              |
| 59:HH:8:ILE:HG21  | 59:HH:28:LEU:HD13  | 2.00                     | 0.44              |
| 48:5:4408:G:C6    | 48:5:4409:C:C4     | 3.06                     | 0.44              |
| 48:5:4232:U:H1'   | 48:5:4233:A:OP2    | 2.18                     | 0.44              |
| 67:PP:34:MET:HE2  | 67:PP:42:ARG:HA    | 1.99                     | 0.44              |
| 50:8:68:G:H2'     | 50:8:69:U:O4'      | 2.17                     | 0.44              |
| 48:5:4240:G:C6    | 48:5:4241:C:C4     | 3.05                     | 0.44              |
| 59:HH:66:VAL:HB   | 59:HH:67:PRO:HD3   | 2.00                     | 0.44              |
| 15:P:18:ARG:HA    | 15:P:147:GLU:HA    | 1.99                     | 0.44              |
| 51:9:1307:U:C3'   | 51:9:1308:U:H5''   | 2.46                     | 0.44              |
| 51:9:668:A:N1     | 51:9:1143:A:C5     | 2.86                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:9:752:G:C2      | 51:9:790:C:N3     | 2.85                     | 0.44              |
| 51:9:832:G:C6      | 51:9:833:C:C4     | 3.06                     | 0.44              |
| 51:9:1551:U:O2     | 51:9:1551:U:O4'   | 2.35                     | 0.44              |
| 51:9:1559:C:C2     | 51:9:1577:G:N2    | 2.85                     | 0.44              |
| 50:8:126:C:O2'     | 50:8:127:U:C5     | 2.64                     | 0.44              |
| 48:5:207:G:C6      | 48:5:208:A:C6     | 3.05                     | 0.44              |
| 51:9:1749:G:C6     | 51:9:1750:C:C4    | 3.06                     | 0.44              |
| 48:5:2898:G:C2     | 48:5:2899:C:C2    | 3.05                     | 0.44              |
| 50:8:134:G:C2      | 50:8:135:C:C2     | 3.06                     | 0.44              |
| 51:9:1623:A:H5''   | 70:SS:133:GLY:HA3 | 2.00                     | 0.44              |
| 50:8:60:G:O6       | 50:8:96:C:O2'     | 2.25                     | 0.44              |
| 48:5:977:C:C3'     | 48:5:978:G:H5'    | 2.46                     | 0.44              |
| 17:R:99:MET:O      | 17:R:103:ARG:HB2  | 2.17                     | 0.44              |
| 51:9:993:G:OP1     | 51:9:1131:G:N2    | 2.40                     | 0.44              |
| 48:5:1270:A:C5     | 48:5:1271:G:H1'   | 2.53                     | 0.44              |
| 48:5:2088:A:O2'    | 48:5:2089:G:P     | 2.76                     | 0.44              |
| 48:5:1404:G:C2     | 48:5:1405:C:C2    | 3.06                     | 0.44              |
| 51:9:1500:G:C6     | 51:9:1501:C:N3    | 2.86                     | 0.44              |
| 48:5:4147:G:C6     | 48:5:4148:C:C4    | 3.05                     | 0.44              |
| 51:9:964:A:N3      | 51:9:1054:G:O2'   | 2.45                     | 0.44              |
| 51:9:187:G:C2      | 51:9:188:C:C2     | 3.05                     | 0.44              |
| 48:5:2270:G:C2     | 48:5:2271:C:C2    | 3.06                     | 0.44              |
| 48:5:2021:G:C6     | 48:5:2022:C:C4    | 3.06                     | 0.44              |
| 48:5:1374:G:C6     | 48:5:1375:C:C4    | 3.06                     | 0.44              |
| 52:AA:124:VAL:HG13 | 52:AA:130:ASP:HB2 | 1.99                     | 0.44              |
| 48:5:2:G:C2        | 48:5:3:C:C2       | 3.06                     | 0.44              |
| 60:II:6:ASP:N      | 60:II:6:ASP:OD1   | 2.51                     | 0.44              |
| 51:9:1345:G:OP1    | 51:9:1688:C:O2'   | 2.36                     | 0.44              |
| 48:5:4216:G:C2'    | 48:5:4217:G:H5'   | 2.48                     | 0.44              |
| 51:9:696:G:C2      | 51:9:735:C:C2     | 3.06                     | 0.44              |
| 3:C:28:PHE:HA      | 3:C:129:ALA:HA    | 2.00                     | 0.44              |
| 48:5:4508:C:N3     | 48:5:4512:U:H5    | 2.16                     | 0.44              |
| 5:E:132:HIS:CE1    | 48:5:711:A:H1'    | 2.53                     | 0.44              |
| 48:5:2793:G:H5''   | 48:5:2794:C:H5''  | 1.99                     | 0.43              |
| 48:5:3861:A:H2'    | 48:5:3862:A:C8    | 2.53                     | 0.43              |
| 51:9:92:A:H2'      | 51:9:446:G:N2     | 2.32                     | 0.43              |
| 2:B:154:LYS:CB     | 2:B:154:LYS:NZ    | 2.81                     | 0.43              |
| 19:T:85:LEU:HD13   | 48:5:4305:G:C2    | 2.53                     | 0.43              |
| 59:HH:43:LEU:HD22  | 59:HH:72:PHE:CD2  | 2.53                     | 0.43              |
| 51:9:379:C:N3      | 60:II:5:ARG:NH1   | 2.66                     | 0.43              |
| 48:5:4890:G:C2     | 48:5:4930:C:C2    | 3.06                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 69:RR:38:ILE:HD12 | 69:RR:39:ALA:N    | 2.33                     | 0.43              |
| 51:9:1777:G:C6    | 51:9:1778:C:C4    | 3.06                     | 0.43              |
| 48:5:2612:G:C6    | 48:5:2613:C:C4    | 3.05                     | 0.43              |
| 68:QQ:84:ILE:HG13 | 68:QQ:85:ARG:N    | 2.32                     | 0.43              |
| 51:9:1664:A:HO2'  | 51:9:1665:G:C5'   | 2.30                     | 0.43              |
| 53:BB:189:ILE:HB  | 53:BB:190:PRO:HD3 | 1.99                     | 0.43              |
| 48:5:4713:G:C6    | 48:5:4714:C:C4    | 3.05                     | 0.43              |
| 51:9:1847:G:C2    | 51:9:1853:C:C2    | 3.06                     | 0.43              |
| 17:R:99:MET:SD    | 17:R:99:MET:N     | 2.91                     | 0.43              |
| 48:5:1874:A:C5'   | 48:5:4218:U:O2    | 2.66                     | 0.43              |
| 48:5:1280:C:C2    | 48:5:1282:G:C4    | 3.06                     | 0.43              |
| 2:B:261:ARG:HB2   | 14:O:64:THR:HG21  | 2.00                     | 0.43              |
| 48:5:1265:G:OP1   | 48:5:2115:G:N1    | 2.51                     | 0.43              |
| 3:C:262:ASP:O     | 3:C:271:ALA:O     | 2.36                     | 0.43              |
| 48:5:2654:C:N3    | 48:5:2681:G:C2    | 2.86                     | 0.43              |
| 2:B:56:ILE:CG1    | 2:B:365:LEU:HD22  | 2.47                     | 0.43              |
| 51:9:1315:U:C4    | 51:9:1316:C:C4    | 3.06                     | 0.43              |
| 48:5:2567:G:C6    | 48:5:2568:C:C4    | 3.07                     | 0.43              |
| 51:9:1337:C:O2'   | 72:UU:68:THR:HG23 | 2.18                     | 0.43              |
| 48:5:5:A:C6       | 48:5:6:C:C4       | 3.07                     | 0.43              |
| 48:5:3610:A:O2'   | 60:II:89:GLU:OE1  | 2.19                     | 0.43              |
| 51:9:623:G:N2     | 51:9:624:C:C2     | 2.86                     | 0.43              |
| 48:5:4681:A:H2'   | 48:5:4682:U:O4'   | 2.18                     | 0.43              |
| 48:5:4139:G:C6    | 48:5:4140:C:C4    | 3.06                     | 0.43              |
| 51:9:29:G:C2      | 51:9:30:C:C2      | 3.06                     | 0.43              |
| 48:5:4666:G:C2    | 48:5:4667:C:C2    | 3.06                     | 0.43              |
| 48:5:4320:G:H2'   | 48:5:4321:U:O4'   | 2.18                     | 0.43              |
| 48:5:4142:C:C4    | 48:5:4143:G:N1    | 2.86                     | 0.43              |
| 48:5:1436:C:O5'   | 48:5:2119:C:N4    | 2.51                     | 0.43              |
| 1:A:34:PHE:CD2    | 48:5:4087:G:C6    | 3.06                     | 0.43              |
| 47:3:69:G:O2'     | 47:3:70:G:C8      | 2.70                     | 0.43              |
| 48:5:4482:U:N3    | 48:5:4483:C:C5    | 2.86                     | 0.43              |
| 60:II:182:CYS:SG  | 60:II:183:GLY:N   | 2.92                     | 0.43              |
| 51:9:114:G:O6     | 51:9:351:G:H1'    | 2.18                     | 0.43              |
| 48:5:1925:G:C2    | 48:5:1926:C:C2    | 3.06                     | 0.43              |
| 51:9:1777:G:C2    | 51:9:1778:C:C2    | 3.05                     | 0.43              |
| 23:X:119:ILE:HG23 | 23:X:120:ASP:N    | 2.33                     | 0.43              |
| 14:O:48:TYR:CE2   | 48:5:1930:U:C2    | 3.07                     | 0.43              |
| 8:H:117:PHE:CE1   | 8:H:118:LEU:HD23  | 2.53                     | 0.43              |
| 48:5:1237:C:O4'   | 48:5:1237:C:O2    | 2.33                     | 0.43              |
| 51:9:1524:G:N2    | 51:9:1525:C:C2    | 2.87                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:2703:G:C2     | 48:5:2704:C:C2     | 3.06                     | 0.43              |
| 53:BB:125:VAL:HG22 | 53:BB:169:MET:HG3  | 2.00                     | 0.43              |
| 65:NN:88:LEU:CD2   | 65:NN:135:LEU:HD11 | 2.48                     | 0.43              |
| 51:9:14:C:O2       | 51:9:1198:G:C2     | 2.72                     | 0.43              |
| 48:5:254:G:C2      | 48:5:255:C:C2      | 3.06                     | 0.43              |
| 48:5:952:G:C6      | 48:5:953:C:C4      | 3.06                     | 0.43              |
| 48:5:1090:G:C2     | 48:5:1091:C:C2     | 3.06                     | 0.43              |
| 48:5:3590:G:N1     | 48:5:3591:C:C2     | 2.86                     | 0.43              |
| 51:9:1643:U:H2'    | 51:9:1644:C:H6     | 1.83                     | 0.43              |
| 48:5:2457:G:C6     | 48:5:2458:C:C4     | 3.06                     | 0.43              |
| 56:EE:72:ILE:HD13  | 56:EE:82:TYR:CD1   | 2.53                     | 0.43              |
| 48:5:1655:C:H2'    | 48:5:1656:U:H5''   | 2.00                     | 0.43              |
| 48:5:2871:A:H2'    | 48:5:2872:C:O4'    | 2.18                     | 0.43              |
| 60:II:38:ILE:HD11  | 60:II:81:VAL:HG23  | 2.00                     | 0.43              |
| 7:G:30:PRO:HG2     | 7:G:31:LEU:HD22    | 2.00                     | 0.43              |
| 11:L:163:LYS:NZ    | 48:5:509:A:H5'     | 2.33                     | 0.43              |
| 48:5:76:A:C5       | 48:5:77:U:C5       | 3.07                     | 0.43              |
| 48:5:1724:G:C4'    | 48:5:1725:U:OP2    | 2.63                     | 0.43              |
| 48:5:1270:A:C2'    | 48:5:1271:G:O5'    | 2.66                     | 0.43              |
| 4:D:44:TYR:CD1     | 48:5:1823:G:H4'    | 2.54                     | 0.43              |
| 3:C:86:ARG:HA      | 3:C:89:GLN:HG3     | 2.00                     | 0.43              |
| 48:5:476:G:C2      | 48:5:679:C:C2      | 3.06                     | 0.43              |
| 48:5:2463:G:C2     | 48:5:2464:C:C2     | 3.07                     | 0.43              |
| 51:9:1335:G:C2     | 51:9:1336:C:C2     | 3.05                     | 0.43              |
| 48:5:2559:G:C2     | 48:5:2560:C:C2     | 3.06                     | 0.43              |
| 48:5:4240:G:C2     | 48:5:4241:C:C2     | 3.06                     | 0.43              |
| 48:5:2612:G:C2     | 48:5:2613:C:C2     | 3.06                     | 0.43              |
| 48:5:4666:G:C6     | 48:5:4667:C:C4     | 3.05                     | 0.43              |
| 8:H:117:PHE:CZ     | 8:H:118:LEU:HD23   | 2.54                     | 0.43              |
| 53:BB:136:ARG:HG3  | 53:BB:136:ARG:HH21 | 1.82                     | 0.43              |
| 48:5:1048:G:C6     | 48:5:1049:C:C4     | 3.06                     | 0.43              |
| 61:JJ:128:VAL:O    | 61:JJ:132:GLN:HG3  | 2.19                     | 0.43              |
| 51:9:1246:A:N3     | 51:9:1251:A:O2'    | 2.46                     | 0.43              |
| 52:AA:33:GLN:HB3   | 52:AA:154:LEU:HD12 | 2.01                     | 0.43              |
| 60:II:44:HIS:O     | 60:II:56:ARG:N     | 2.51                     | 0.43              |
| 47:3:41:U:C4'      | 57:FF:198:ARG:HD3  | 2.48                     | 0.43              |
| 48:5:744:G:C2      | 48:5:921:C:C2      | 3.06                     | 0.43              |
| 51:9:1109:C:C2'    | 51:9:1109:C:O2     | 2.63                     | 0.43              |
| 48:5:1271:G:H3'    | 48:5:1272:C:H5'    | 2.00                     | 0.43              |
| 63:LL:77:VAL:HA    | 63:LL:88:ILE:HG22  | 2.01                     | 0.43              |
| 46:2:35:A:OP2      | 68:QQ:146:ARG:NH1  | 2.51                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:LL:5:GLN:OE1    | 63:LL:11:GLN:HB2   | 2.18                     | 0.43              |
| 57:FF:99:ILE:HD13  | 57:FF:171:GLU:HA   | 2.00                     | 0.43              |
| 48:5:1048:G:C2     | 48:5:1049:C:C2     | 3.05                     | 0.43              |
| 51:9:1121:G:C6     | 51:9:1122:A:C5     | 3.06                     | 0.43              |
| 23:X:96:LEU:HG     | 23:X:140:LEU:HD11  | 1.99                     | 0.43              |
| 3:C:342:ARG:HG3    | 3:C:342:ARG:HH11   | 1.84                     | 0.43              |
| 70:SS:28:PHE:O     | 70:SS:31:THR:OG1   | 2.36                     | 0.43              |
| 46:2:65:G:N2       | 46:2:66:C:C2       | 2.87                     | 0.43              |
| 48:5:4250:G:C2     | 48:5:4259:C:C2     | 3.06                     | 0.43              |
| 52:AA:119:PRO:HG2  | 52:AA:142:LEU:HD11 | 2.00                     | 0.43              |
| 7:G:87:LEU:HD11    | 7:G:91:THR:HG21    | 2.01                     | 0.43              |
| 48:5:1358:G:N3     | 48:5:1359:G:N7     | 2.66                     | 0.43              |
| 51:9:1455:A:H2'    | 51:9:1456:G:H8     | 1.84                     | 0.43              |
| 54:CC:192:LEU:HD12 | 54:CC:193:VAL:N    | 2.33                     | 0.43              |
| 48:5:1213:G:C6     | 48:5:1215:C:C4     | 3.06                     | 0.43              |
| 51:9:65:C:C2       | 58:GG:174:PRO:HB3  | 2.54                     | 0.43              |
| 48:5:642:G:C2      | 48:5:643:C:C4      | 3.06                     | 0.43              |
| 47:3:33:U:C5'      | 57:FF:127:ARG:NH1  | 2.82                     | 0.43              |
| 51:9:522:A:H4'     | 61:JJ:131:ARG:HH22 | 1.84                     | 0.43              |
| 60:II:25:ARG:HB3   | 60:II:27:TYR:CE2   | 2.54                     | 0.43              |
| 48:5:2481:G:C2     | 48:5:2482:C:C2     | 3.07                     | 0.43              |
| 48:5:469:C:C2      | 48:5:470:A:C8      | 3.07                     | 0.43              |
| 2:B:43:LEU:HD13    | 2:B:196:TRP:HH2    | 1.82                     | 0.43              |
| 48:5:1811:G:C2     | 48:5:1812:C:C2     | 3.07                     | 0.43              |
| 48:5:298:G:C2      | 48:5:299:C:C2      | 3.07                     | 0.43              |
| 48:5:4904:G:C2     | 48:5:4905:C:C2     | 3.06                     | 0.43              |
| 51:9:1492:U:H1'    | 72:UU:70:CYS:SG    | 2.58                     | 0.43              |
| 58:GG:76:LEU:HD22  | 58:GG:92:ARG:HG2   | 2.00                     | 0.43              |
| 51:9:29:G:C6       | 51:9:30:C:C4       | 3.06                     | 0.43              |
| 13:N:180:PHE:O     | 13:N:182:HIS:N     | 2.52                     | 0.43              |
| 48:5:4187:G:H2'    | 48:5:4188:U:O4'    | 2.19                     | 0.43              |
| 48:5:2862:G:N3     | 48:5:3624:A:H2'    | 2.34                     | 0.43              |
| 48:5:3705:G:C6     | 48:5:3706:C:C4     | 3.06                     | 0.43              |
| 51:9:839:C:C2'     | 51:9:839:C:O2      | 2.65                     | 0.43              |
| 48:5:4222:G:C6     | 48:5:4223:C:C4     | 3.07                     | 0.43              |
| 48:5:2816:G:C6     | 48:5:2817:C:C4     | 3.06                     | 0.43              |
| 3:C:224:ILE:HG22   | 3:C:227:ILE:HD13   | 1.99                     | 0.43              |
| 48:5:4349:C:H3'    | 48:5:4350:C:C5'    | 2.48                     | 0.43              |
| 9:I:191:ILE:HD12   | 9:I:200:ILE:HD12   | 1.56                     | 0.43              |
| 51:9:911:C:C3'     | 51:9:912:C:H5'     | 2.47                     | 0.43              |
| 48:5:744:G:H2'     | 48:5:745:G:H8      | 1.83                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:5:4919:G:N2    | 48:5:4920:C:C2     | 2.87                     | 0.43              |
| 48:5:199:G:C2     | 48:5:201:C:C4      | 3.06                     | 0.43              |
| 51:9:1728:U:H3'   | 51:9:1729:U:H5''   | 2.01                     | 0.43              |
| 48:5:2256:C:H1'   | 48:5:2257:C:OP2    | 2.19                     | 0.43              |
| 51:9:1398:G:N1    | 51:9:1399:C:C4     | 2.87                     | 0.43              |
| 48:5:1912:G:C2    | 48:5:1913:C:C2     | 3.07                     | 0.43              |
| 2:B:114:CYS:SG    | 2:B:180:LEU:HD11   | 2.59                     | 0.43              |
| 48:5:4129:G:C2    | 48:5:4130:C:C2     | 3.06                     | 0.43              |
| 51:9:1229:G:C6    | 51:9:1230:C:C4     | 3.07                     | 0.43              |
| 16:Q:89:ASP:OD1   | 16:Q:91:ARG:NH2    | 2.51                     | 0.43              |
| 75:XX:84:PHE:HB2  | 75:XX:118:VAL:HG11 | 1.99                     | 0.43              |
| 2:B:2:SER:N       | 48:5:4517:A:OP2    | 2.52                     | 0.43              |
| 68:QQ:41:MET:SD   | 68:QQ:41:MET:N     | 2.91                     | 0.43              |
| 48:5:322:C:O2     | 48:5:4356:G:C2     | 2.71                     | 0.43              |
| 48:5:1959:U:OP1   | 48:5:1960:A:O3'    | 2.37                     | 0.43              |
| 48:5:1929:A:C2    | 48:5:2054:U:O4     | 2.60                     | 0.43              |
| 48:5:1280:C:C4    | 48:5:1282:G:O6     | 2.72                     | 0.43              |
| 51:9:1406:G:C4    | 51:9:1407:U:H1'    | 2.54                     | 0.43              |
| 48:5:2793:G:C6    | 48:5:2797:C:N4     | 2.86                     | 0.43              |
| 56:EE:153:LEU:O   | 56:EE:155:LYS:HD3  | 2.19                     | 0.43              |
| 47:3:39:U:HO2'    | 47:3:40:C:H6       | 1.43                     | 0.43              |
| 60:II:79:ILE:HG23 | 60:II:103:LEU:HB2  | 1.99                     | 0.43              |
| 51:9:1260:A:C4    | 51:9:1620:A:N7     | 2.87                     | 0.43              |
| 48:5:301:G:C2     | 48:5:302:C:C2      | 3.07                     | 0.43              |
| 15:P:36:ILE:CD1   | 15:P:48:LEU:HD11   | 2.49                     | 0.43              |
| 57:FF:20:PHE:HZ   | 57:FF:69:VAL:HG11  | 1.83                     | 0.43              |
| 13:N:50:ARG:NH2   | 48:5:279:A:OP2     | 2.51                     | 0.43              |
| 48:5:1691:G:C2    | 48:5:1692:C:C2     | 3.06                     | 0.43              |
| 48:5:1374:G:C2    | 48:5:1375:C:C2     | 3.07                     | 0.43              |
| 48:5:4274:A:H2'   | 48:5:4275:G:C8     | 2.54                     | 0.43              |
| 48:5:742:G:C2     | 48:5:923:C:C2      | 3.07                     | 0.43              |
| 21:V:20:LEU:HB2   | 21:V:55:ALA:O      | 2.19                     | 0.43              |
| 51:9:1097:G:C6    | 51:9:1098:C:C4     | 3.07                     | 0.43              |
| 1:A:103:PRO:HA    | 1:A:163:ARG:HA     | 1.99                     | 0.43              |
| 48:5:258:G:C2     | 48:5:259:C:C2      | 3.07                     | 0.43              |
| 49:7:93:G:C2      | 49:7:94:C:C2       | 3.07                     | 0.43              |
| 51:9:910:G:C6     | 51:9:911:C:C4      | 3.06                     | 0.43              |
| 51:9:1516:G:O3'   | 67:PP:122:THR:HG21 | 2.19                     | 0.43              |
| 51:9:1143:A:H2'   | 51:9:1144:A:C8     | 2.54                     | 0.43              |
| 47:3:37:A:N1      | 57:FF:133:THR:HG23 | 2.34                     | 0.43              |
| 51:9:981:A:H2'    | 51:9:982:G:C8      | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:9:841:G:N2     | 51:9:842:C:C2     | 2.87                     | 0.43              |
| 11:L:19:GLN:HA    | 11:L:22:VAL:HG23  | 1.99                     | 0.43              |
| 67:PP:20:VAL:HG12 | 67:PP:25:LEU:HG   | 2.01                     | 0.43              |
| 74:WW:75:ILE:HD11 | 74:WW:93:LEU:HD11 | 2.00                     | 0.43              |
| 59:HH:145:ARG:HA  | 74:WW:51:GLU:HB3  | 2.01                     | 0.43              |
| 63:LL:106:HIS:O   | 63:LL:106:HIS:ND1 | 2.52                     | 0.43              |
| 46:2:30:G:N1      | 46:2:31:C:C2      | 2.86                     | 0.43              |
| 22:W:44:ARG:CG    | 22:W:44:ARG:HH11  | 2.32                     | 0.43              |
| 48:5:4911:A:H3'   | 48:5:4912:G:H5''  | 2.01                     | 0.43              |
| 56:EE:72:ILE:HD12 | 56:EE:77:ARG:HB2  | 2.00                     | 0.43              |
| 48:5:3891:A:H2'   | 48:5:3892:U:O4'   | 2.18                     | 0.43              |
| 48:5:4891:G:C2    | 48:5:4929:C:C2    | 3.07                     | 0.43              |
| 48:5:4948:C:H3'   | 48:5:4949:G:N2    | 2.33                     | 0.43              |
| 13:N:94:PHE:CE2   | 13:N:96:ARG:HB2   | 2.54                     | 0.43              |
| 50:8:118:C:C2     | 50:8:133:G:C2     | 3.06                     | 0.43              |
| 48:5:1959:U:H4'   | 48:5:1961:G:O4'   | 2.19                     | 0.42              |
| 51:9:1308:U:H2'   | 51:9:1309:C:C1'   | 2.49                     | 0.42              |
| 48:5:1075:G:C6    | 48:5:1076:C:C4    | 3.08                     | 0.42              |
| 6:F:92:ALA:CB     | 6:F:127:LEU:HD21  | 2.49                     | 0.42              |
| 51:9:1568:C:H2'   | 51:9:1569:A:C8    | 2.54                     | 0.42              |
| 48:5:93:G:O2'     | 48:5:94:A:O5'     | 2.37                     | 0.42              |
| 48:5:702:U:H2'    | 48:5:703:G:H4'    | 2.01                     | 0.42              |
| 48:5:3597:G:C6    | 48:5:3598:C:C4    | 3.07                     | 0.42              |
| 50:8:10:G:C6      | 50:8:11:C:C4      | 3.07                     | 0.42              |
| 48:5:2034:G:C6    | 48:5:2035:C:C4    | 3.06                     | 0.42              |
| 48:5:1846:G:C2    | 48:5:1847:C:C2    | 3.07                     | 0.42              |
| 66:OO:38:ASN:HA   | 66:OO:69:SER:OG   | 2.19                     | 0.42              |
| 48:5:2076:G:C6    | 48:5:2077:C:C4    | 3.07                     | 0.42              |
| 50:8:53:G:C6      | 50:8:54:C:C4      | 3.07                     | 0.42              |
| 1:A:13:GLY:HA2    | 48:5:1660:U:H3'   | 71.18                    | 0.42              |
| 48:5:975:C:H5''   | 48:5:976:G:OP2    | 2.20                     | 0.42              |
| 48:5:976:G:C6     | 48:5:977:C:N3     | 2.87                     | 0.42              |
| 10:J:119:TYR:CB   | 70:SS:12:ILE:HG21 | 2.50                     | 0.42              |
| 48:5:1367:C:H1'   | 48:5:1370:G:C8    | 2.54                     | 0.42              |
| 47:3:35:U:H1'     | 51:9:1640:A:O3'   | 2.18                     | 0.42              |
| 48:5:199:G:C4     | 48:5:201:C:C5     | 3.07                     | 0.42              |
| 56:EE:195:ILE:O   | 56:EE:210:VAL:HA  | 2.18                     | 0.42              |
| 48:5:4583:C:N3    | 48:5:4718:G:C2    | 2.88                     | 0.42              |
| 51:9:1335:G:N1    | 51:9:1336:C:C2    | 2.87                     | 0.42              |
| 8:H:5:LEU:HD22    | 8:H:60:TRP:CH2    | 2.54                     | 0.42              |
| 51:9:798:G:O6     | 51:9:861:A:N7     | 2.51                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1664:A:O2'    | 51:9:1665:G:C5'    | 2.68                     | 0.42              |
| 51:9:1664:A:O2'    | 51:9:1665:G:H5'    | 2.20                     | 0.42              |
| 21:V:20:LEU:HD13   | 21:V:26:ILE:HG21   | 2.01                     | 0.42              |
| 1:A:30:ARG:O       | 1:A:163:ARG:NH2    | 2.52                     | 0.42              |
| 48:5:4898:G:N2     | 48:5:4923:C:C2     | 2.87                     | 0.42              |
| 57:FF:179:ASN:HD22 | 57:FF:179:ASN:N    | 2.16                     | 0.42              |
| 61:JJ:24:ARG:HG2   | 61:JJ:24:ARG:HH11  | 1.83                     | 0.42              |
| 66:OO:150:ARG:HB3  | 66:OO:150:ARG:CZ   | 2.49                     | 0.42              |
| 51:9:1439:A:H2'    | 51:9:1440:C:O4'    | 2.19                     | 0.42              |
| 48:5:405:U:O2'     | 48:5:407:A:N7      | 2.39                     | 0.42              |
| 48:5:2358:G:H2'    | 48:5:2359:U:O4'    | 2.19                     | 0.42              |
| 71:TT:28:LEU:O     | 71:TT:29:LYS:HB2   | 2.19                     | 0.42              |
| 48:5:1539:G:C6     | 48:5:1540:C:C4     | 3.06                     | 0.42              |
| 54:CC:166:ARG:HB3  | 54:CC:247:THR:HB   | 2.01                     | 0.42              |
| 5:E:59:TYR:CE2     | 5:E:64:LEU:HD12    | 2.48                     | 0.42              |
| 51:9:912:C:H3'     | 51:9:913:A:C5'     | 2.49                     | 0.42              |
| 51:9:1268:C:C2     | 51:9:1515:G:N2     | 2.88                     | 0.42              |
| 48:5:504:G:H22     | 48:5:654:C:H1'     | 1.84                     | 0.42              |
| 51:9:1454:A:OP1    | 69:RR:3:ARG:HG2    | 2.19                     | 0.42              |
| 51:9:156:G:H4'     | 58:GG:108:VAL:HG23 | 2.00                     | 0.42              |
| 51:9:522:A:C3'     | 61:JJ:131:ARG:HH22 | 2.32                     | 0.42              |
| 51:9:833:C:H4'     | 51:9:834:C:OP1     | 2.19                     | 0.42              |
| 51:9:1613:G:N2     | 51:9:1627:C:C2     | 2.88                     | 0.42              |
| 2:B:378:ARG:NE     | 22:W:32:LEU:HD21   | 2.34                     | 0.42              |
| 48:5:1811:G:C6     | 48:5:1812:C:C4     | 3.07                     | 0.42              |
| 51:9:1229:G:C2     | 51:9:1230:C:C2     | 3.07                     | 0.42              |
| 48:5:1584:G:C2     | 48:5:1585:C:C2     | 3.08                     | 0.42              |
| 60:II:156:ALA:O    | 60:II:158:ILE:N    | 2.53                     | 0.42              |
| 48:5:208:A:C6      | 48:5:233:U:C4      | 3.06                     | 0.42              |
| 49:7:110:G:C2      | 49:7:111:C:C2      | 3.06                     | 0.42              |
| 48:5:952:G:C2      | 48:5:953:C:C2      | 3.07                     | 0.42              |
| 4:D:22:ARG:NH1     | 4:D:28:THR:OG1     | 2.53                     | 0.42              |
| 48:5:4395:U:C6     | 48:5:4395:U:H5'    | 2.55                     | 0.42              |
| 51:9:1609:C:H2'    | 51:9:1610:G:C8     | 2.53                     | 0.42              |
| 19:T:40:VAL:HG13   | 19:T:96:ILE:HG23   | 2.01                     | 0.42              |
| 62:KK:64:TRP:O     | 62:KK:65:ARG:C     | 2.57                     | 0.42              |
| 8:H:134:CYS:SG     | 8:H:144:LEU:HD23   | 2.59                     | 0.42              |
| 56:EE:45:ILE:HA    | 56:EE:61:VAL:HG11  | 2.01                     | 0.42              |
| 59:HH:44:ASN:N     | 59:HH:68:GLN:OE1   | 2.52                     | 0.42              |
| 10:J:141:ILE:HD11  | 49:7:55:A:N3       | 2.34                     | 0.42              |
| 51:9:1236:G:C2     | 51:9:1237:C:C2     | 3.07                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:5:3724:A:C6     | 48:5:3725:G:C5    | 3.08                     | 0.42              |
| 48:5:4920:C:H2'    | 48:5:4921:C:C6    | 2.55                     | 0.42              |
| 48:5:2712:G:N1     | 48:5:2713:C:C4    | 2.87                     | 0.42              |
| 48:5:1781:U:C4     | 48:5:1782:U:C5    | 3.08                     | 0.42              |
| 48:5:4462:C:C2     | 48:5:4515:G:N2    | 2.87                     | 0.42              |
| 48:5:4152:G:C2     | 48:5:4153:C:C2    | 3.08                     | 0.42              |
| 48:5:4737:G:C6     | 48:5:4738:C:C4    | 3.07                     | 0.42              |
| 48:5:2076:G:C2     | 48:5:2077:C:C2    | 3.08                     | 0.42              |
| 48:5:2606:G:C2     | 48:5:2607:C:C2    | 3.07                     | 0.42              |
| 24:Y:55:VAL:HG13   | 24:Y:104:VAL:HG13 | 2.02                     | 0.42              |
| 6:F:175:ALA:O      | 6:F:179:ARG:HB2   | 2.19                     | 0.42              |
| 48:5:1431:C:C2     | 48:5:1454:G:C2    | 3.06                     | 0.42              |
| 48:5:1431:C:C2     | 48:5:1454:G:N2    | 2.87                     | 0.42              |
| 5:E:43:ASN:HB3     | 5:E:58:MET:SD     | 2.59                     | 0.42              |
| 51:9:1566:G:N7     | 71:TT:101:ARG:NH2 | 2.65                     | 0.42              |
| 52:AA:3:GLY:N      | 73:VV:78:ILE:O    | 2.52                     | 0.42              |
| 48:5:2468:U:C2     | 48:5:2473:A:N6    | 2.85                     | 0.42              |
| 48:5:3751:G:HO2'   | 48:5:3752:C:H5'   | 1.77                     | 0.42              |
| 48:5:3753:G:O2'    | 48:5:3754:G:H5'   | 2.20                     | 0.42              |
| 3:C:114:ARG:HB3    | 13:N:203:TYR:CD1  | 2.54                     | 0.42              |
| 48:5:4371:G:C5     | 48:5:4372:U:C4    | 3.07                     | 0.42              |
| 56:EE:151:ASP:O    | 56:EE:153:LEU:N   | 2.52                     | 0.42              |
| 48:5:199:G:C2      | 48:5:201:C:C2     | 3.07                     | 0.42              |
| 56:EE:126:VAL:HG23 | 56:EE:157:ASN:H   | 1.84                     | 0.42              |
| 6:F:92:ALA:HB3     | 6:F:127:LEU:HD21  | 2.00                     | 0.42              |
| 3:C:86:ARG:HD3     | 48:5:376:A:OP1    | 2.19                     | 0.42              |
| 48:5:2712:G:C2     | 48:5:2713:C:C2    | 3.08                     | 0.42              |
| 48:5:1205:G:C2     | 48:5:1206:C:C2    | 3.08                     | 0.42              |
| 51:9:211:G:C6      | 51:9:212:C:N4     | 2.88                     | 0.42              |
| 48:5:5031:G:C6     | 48:5:5032:C:C4    | 3.08                     | 0.42              |
| 48:5:2609:G:N1     | 48:5:2731:C:C2    | 2.88                     | 0.42              |
| 48:5:1755:C:C3'    | 48:5:1756:U:H5''  | 2.50                     | 0.42              |
| 50:8:139:G:C2      | 50:8:140:C:C2     | 3.08                     | 0.42              |
| 14:O:48:TYR:CE2    | 14:O:52:LEU:HD11  | 2.54                     | 0.42              |
| 51:9:839:C:O2      | 51:9:839:C:H2'    | 2.17                     | 0.42              |
| 48:5:1466:G:N2     | 48:5:1467:C:C2    | 2.88                     | 0.42              |
| 10:J:15:LEU:HD11   | 10:J:157:ILE:HG23 | 2.01                     | 0.42              |
| 48:5:4931:G:H2'    | 48:5:4931:G:N3    | 2.35                     | 0.42              |
| 48:5:963:G:H2'     | 48:5:963:G:N3     | 2.35                     | 0.42              |
| 47:3:4:C:O2        | 47:3:4:C:H2'      | 2.20                     | 0.42              |
| 55:DD:31:GLU:OE1   | 55:DD:106:ARG:NH2 | 2.52                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 48:5:2526:C:N4   | 48:5:2527:A:N6    | 2.67                     | 0.42              |
| 50:8:31:G:C2     | 50:8:32:C:C2      | 3.08                     | 0.42              |
| 51:9:1189:A:H2'  | 51:9:1190:A:C8    | 2.54                     | 0.42              |
| 51:9:1753:C:C2   | 51:9:1780:G:C2    | 3.07                     | 0.42              |
| 48:5:174:C:C2    | 48:5:263:G:C2     | 3.07                     | 0.42              |
| 11:L:104:ASN:OD1 | 11:L:110:LEU:HB2  | 2.18                     | 0.42              |
| 48:5:165:A:H3'   | 48:5:166:C:H6     | 1.85                     | 0.42              |
| 48:5:1550:G:C2   | 48:5:1579:C:O2    | 2.72                     | 0.42              |
| 48:5:2294:G:N2   | 48:5:2295:C:C2    | 2.87                     | 0.42              |
| 48:5:1075:G:N2   | 48:5:1076:C:C2    | 2.88                     | 0.42              |
| 6:F:92:ALA:HA    | 6:F:147:PRO:HD3   | 2.01                     | 0.42              |
| 51:9:1500:G:C5   | 51:9:1501:C:C4    | 3.06                     | 0.42              |
| 48:5:127:G:C2    | 48:5:128:C:C2     | 3.07                     | 0.42              |
| 48:5:4147:G:C2   | 48:5:4148:C:C2    | 3.07                     | 0.42              |
| 48:5:3712:A:C6   | 51:9:970:G:C2     | 3.08                     | 0.42              |
| 48:5:28:C:C2     | 48:5:55:G:N2      | 2.88                     | 0.42              |
| 51:9:1669:G:C2   | 51:9:1670:C:C2    | 3.07                     | 0.42              |
| 48:5:1557:C:C2   | 48:5:1571:G:C2    | 3.07                     | 0.42              |
| 48:5:2889:G:C6   | 48:5:2890:C:C4    | 3.08                     | 0.42              |
| 48:5:4326:G:C6   | 48:5:4327:C:C4    | 3.08                     | 0.42              |
| 15:P:118:GLN:NE2 | 48:5:423:G:N3     | 2.67                     | 0.42              |
| 48:5:1721:G:C6   | 48:5:1722:C:C4    | 3.08                     | 0.42              |
| 48:5:976:G:OP1   | 48:5:976:G:C4'    | 2.68                     | 0.42              |
| 61:JJ:120:ALA:O  | 61:JJ:121:LYS:CB  | 2.67                     | 0.42              |
| 19:T:3:ASN:ND2   | 48:5:4212:A:N1    | 2.66                     | 0.42              |
| 48:5:2468:U:C4   | 48:5:2473:A:C6    | 3.07                     | 0.42              |
| 48:5:76:A:C6     | 48:5:77:U:C5      | 3.08                     | 0.42              |
| 51:9:113:G:N2    | 51:9:293:C:C2     | 2.88                     | 0.42              |
| 51:9:1416:C:O3'  | 51:9:1417:C:O4'   | 2.38                     | 0.42              |
| 51:9:1771:G:C6   | 51:9:1772:C:N4    | 2.88                     | 0.42              |
| 48:5:1757:U:C2   | 48:5:1758:G:C8    | 3.07                     | 0.42              |
| 51:9:167:G:N2    | 51:9:168:C:C2     | 2.88                     | 0.42              |
| 48:5:5028:G:C2   | 48:5:5029:C:C2    | 3.07                     | 0.42              |
| 48:5:479:G:C6    | 48:5:480:C:C4     | 3.08                     | 0.42              |
| 51:9:1847:G:N2   | 51:9:1853:C:C2    | 2.88                     | 0.42              |
| 5:E:116:ASP:N    | 5:E:116:ASP:OD1   | 2.52                     | 0.42              |
| 51:9:1604:G:C6   | 51:9:1605:G:C4    | 3.07                     | 0.42              |
| 51:9:1648:G:C8   | 68:QQ:125:ARG:HB3 | 2.54                     | 0.42              |
| 51:9:1804:U:H2'  | 51:9:1805:G:O4'   | 2.20                     | 0.42              |
| 48:5:3923:A:H2'  | 48:5:3924:C:C6    | 2.55                     | 0.42              |
| 48:5:2050:G:C6   | 48:5:2051:C:C4    | 3.07                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:2542:G:C2    | 48:5:2775:C:C2    | 3.07                     | 0.42              |
| 24:Y:19:PHE:O     | 24:Y:26:ARG:NH2   | 2.52                     | 0.42              |
| 48:5:674:G:C2     | 48:5:675:C:C2     | 3.08                     | 0.42              |
| 13:N:4:TYR:OH     | 48:5:151:G:OP2    | 2.23                     | 0.42              |
| 51:9:47:G:C2      | 51:9:48:C:C2      | 3.08                     | 0.42              |
| 51:9:559:G:O2'    | 51:9:560:A:O4'    | 2.37                     | 0.42              |
| 11:L:146:LEU:HB2  | 11:L:148:THR:HG22 | 2.01                     | 0.42              |
| 51:9:799:U:H5''   | 59:HH:110:THR:HB  | 2.02                     | 0.42              |
| 48:5:4072:C:H2'   | 48:5:4073:A:O4'   | 2.20                     | 0.42              |
| 48:5:978:G:OP2    | 48:5:979:C:OP2    | 2.37                     | 0.42              |
| 48:5:4212:A:C2    | 48:5:4218:U:C5    | 3.07                     | 0.42              |
| 48:5:77:U:N3      | 48:5:335:A:C6     | 2.86                     | 0.42              |
| 51:9:595:U:H2'    | 51:9:596:U:C6     | 2.54                     | 0.42              |
| 51:9:1212:G:O2'   | 51:9:1213:C:C5'   | 2.68                     | 0.42              |
| 48:5:3870:C:C2    | 48:5:3886:G:N2    | 2.87                     | 0.42              |
| 48:5:3868:G:N2    | 48:5:3900:G:O2'   | 2.53                     | 0.42              |
| 48:5:3590:G:C6    | 48:5:3591:C:C4    | 3.07                     | 0.42              |
| 19:T:109:VAL:HG13 | 48:5:1803:G:C6    | 2.54                     | 0.42              |
| 1:A:196:TRP:CG    | 1:A:197:PRO:N     | 2.86                     | 0.42              |
| 48:5:1072:C:H1'   | 48:5:1073:G:C8    | 2.54                     | 0.42              |
| 7:G:63:LEU:HD12   | 13:N:32:GLN:HB3   | 2.02                     | 0.42              |
| 48:5:179:G:C6     | 48:5:180:C:C4     | 3.07                     | 0.42              |
| 48:5:742:G:N2     | 48:5:923:C:C2     | 2.88                     | 0.42              |
| 49:7:93:G:C6      | 49:7:94:C:C4      | 3.07                     | 0.42              |
| 51:9:949:G:C2     | 51:9:950:C:C2     | 3.08                     | 0.42              |
| 51:9:978:G:C6     | 51:9:979:C:C4     | 3.08                     | 0.42              |
| 18:S:95:ARG:HD3   | 18:S:97:TYR:OH    | 2.19                     | 0.42              |
| 51:9:163:U:OP1    | 58:GG:84:TYR:HA   | 2.20                     | 0.42              |
| 51:9:999:G:C2     | 51:9:1000:C:C2    | 3.08                     | 0.42              |
| 48:5:691:C:H2'    | 48:5:692:A:C8     | 2.55                     | 0.42              |
| 60:II:106:SER:HB2 | 60:II:166:PHE:CD1 | 2.54                     | 0.42              |
| 48:5:1349:G:C6    | 48:5:1350:C:C4    | 3.08                     | 0.42              |
| 48:5:29:G:C2      | 48:5:30:C:C2      | 3.08                     | 0.42              |
| 48:5:4269:G:C2    | 48:5:4270:C:C2    | 3.08                     | 0.42              |
| 47:3:69:G:O2'     | 47:3:70:G:O5'     | 2.37                     | 0.42              |
| 51:9:910:G:C2     | 51:9:911:C:C2     | 3.08                     | 0.42              |
| 48:5:1359:G:C5    | 48:5:1360:G:C5    | 3.07                     | 0.42              |
| 48:5:2793:G:O6    | 48:5:2797:C:C5    | 2.73                     | 0.42              |
| 58:GG:3:LEU:O     | 58:GG:15:LEU:HA   | 2.20                     | 0.42              |
| 48:5:301:G:C5     | 48:5:302:C:C4     | 3.08                     | 0.42              |
| 13:N:68:ARG:HG2   | 48:5:302:C:OP1    | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:707:C:H42     | 48:5:1290:G:H1     | 1.68                     | 0.42              |
| 51:9:145:G:N1      | 51:9:146:G:C6      | 2.88                     | 0.42              |
| 48:5:4094:G:H2'    | 48:5:4095:G:C1'    | 2.50                     | 0.42              |
| 48:5:2042:A:N3     | 48:5:4462:C:O2'    | 2.49                     | 0.42              |
| 73:VV:32:ILE:O     | 73:VV:54:ALA:HA    | 2.19                     | 0.42              |
| 51:9:1664:A:O2'    | 51:9:1665:G:O5'    | 2.33                     | 0.42              |
| 51:9:1686:G:C2     | 51:9:1687:C:C2     | 3.07                     | 0.42              |
| 48:5:196:C:C2      | 48:5:246:G:C2      | 3.08                     | 0.42              |
| 50:8:2:G:H2'       | 50:8:2:G:N3        | 2.34                     | 0.42              |
| 48:5:1819:G:H5''   | 48:5:1819:G:C8     | 2.55                     | 0.42              |
| 51:9:1089:G:C6     | 51:9:1090:C:C4     | 3.08                     | 0.42              |
| 48:5:4595:G:C6     | 48:5:4596:C:C4     | 3.08                     | 0.42              |
| 12:M:55:MET:O      | 18:S:157:ARG:NH2   | 2.53                     | 0.42              |
| 5:E:149:LEU:HD11   | 5:E:191:ILE:HG13   | 2.01                     | 0.42              |
| 48:5:2645:G:C6     | 48:5:2646:C:C4     | 3.07                     | 0.42              |
| 55:DD:208:VAL:HG21 | 69:RR:50:ILE:HD11  | 2.01                     | 0.42              |
| 57:FF:162:ALA:HB1  | 57:FF:169:ILE:HD13 | 2.01                     | 0.42              |
| 48:5:2831:G:C2     | 48:5:3855:C:C2     | 3.08                     | 0.42              |
| 51:9:52:G:C6       | 51:9:53:C:C4       | 3.07                     | 0.42              |
| 48:5:1806:G:C2     | 48:5:1807:C:C2     | 3.08                     | 0.42              |
| 75:XX:29:LYS:HD3   | 75:XX:35:ALA:HB2   | 2.01                     | 0.42              |
| 51:9:947:G:C2      | 51:9:948:C:C2      | 3.08                     | 0.42              |
| 25:Z:38:TYR:CE1    | 25:Z:76:ASN:OD1    | 2.73                     | 0.42              |
| 51:9:872:A:N6      | 51:9:915:G:C4      | 2.88                     | 0.42              |
| 51:9:830:A:C6      | 51:9:845:G:C4      | 3.08                     | 0.42              |
| 51:9:293:C:O2      | 51:9:293:C:C2'     | 2.68                     | 0.42              |
| 50:8:56:G:C4       | 50:8:62:A:C2       | 3.08                     | 0.42              |
| 3:C:161:TYR:HD1    | 3:C:166:GLU:OE2    | 2.02                     | 0.42              |
| 1:A:207:VAL:HG12   | 48:5:3919:C:C5'    | 2.50                     | 0.42              |
| 4:D:64:ILE:CD1     | 4:D:109:LEU:HD22   | 2.50                     | 0.42              |
| 11:L:29:PRO:CB     | 48:5:1371:A:H2'    | 2.50                     | 0.42              |
| 48:5:3717:A:O2'    | 48:5:3718:A:O5'    | 2.38                     | 0.42              |
| 48:5:4583:C:C2     | 48:5:4718:G:C2     | 3.08                     | 0.42              |
| 48:5:1448:G:C6     | 48:5:1449:C:C4     | 3.08                     | 0.42              |
| 48:5:4093:G:C6     | 48:5:4094:G:N7     | 2.88                     | 0.42              |
| 51:9:67:C:OP2      | 58:GG:132:ARG:NH1  | 2.53                     | 0.42              |
| 5:E:208:LEU:HA     | 5:E:212:TYR:HD2    | 1.84                     | 0.42              |
| 48:5:479:G:C2      | 48:5:480:C:C2      | 3.07                     | 0.42              |
| 48:5:1416:G:C2     | 48:5:1417:C:C2     | 3.07                     | 0.42              |
| 14:O:27:VAL:HG13   | 14:O:98:ALA:HB1    | 2.01                     | 0.42              |
| 48:5:2606:G:C6     | 48:5:2607:C:C4     | 3.08                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:8:32:C:H2'      | 50:8:33:G:O4'      | 2.20                     | 0.42              |
| 54:CC:274:VAL:HG13 | 54:CC:274:VAL:O    | 2.20                     | 0.42              |
| 58:GG:58:LYS:O     | 58:GG:59:GLN:HB2   | 2.20                     | 0.42              |
| 6:F:164:ILE:HB     | 6:F:169:ILE:HD12   | 2.02                     | 0.42              |
| 48:5:235:A:C2      | 48:5:238:C:C5      | 3.08                     | 0.42              |
| 7:G:157:ILE:HG23   | 7:G:167:VAL:HG11   | 2.01                     | 0.42              |
| 55:DD:115:VAL:HG13 | 55:DD:138:VAL:HG11 | 2.01                     | 0.42              |
| 17:R:4:LEU:HD11    | 17:R:29:THR:HG23   | 2.02                     | 0.41              |
| 11:L:42:ARG:CG     | 11:L:45:ARG:HH12   | 2.34                     | 0.41              |
| 47:3:66:U:C4       | 47:3:67:U:C5       | 3.08                     | 0.41              |
| 47:3:69:G:O2'      | 47:3:70:G:P        | 2.78                     | 0.41              |
| 51:9:912:C:H3'     | 51:9:913:A:H5''    | 2.01                     | 0.41              |
| 48:5:1969:G:O2'    | 48:5:1970:A:C5'    | 2.66                     | 0.41              |
| 48:5:1277:G:C2     | 48:5:1278:C:C2     | 3.08                     | 0.41              |
| 48:5:1358:G:O6     | 48:5:1379:C:N3     | 2.52                     | 0.41              |
| 51:9:1344:A:N6     | 51:9:1386:A:H5''   | 2.35                     | 0.41              |
| 5:E:157:ARG:NH2    | 12:M:106:ASP:OD2   | 2.53                     | 0.41              |
| 48:5:2623:A:C2     | 48:5:2624:G:C6     | 3.08                     | 0.41              |
| 51:9:1212:G:O2'    | 51:9:1213:C:P      | 2.78                     | 0.41              |
| 48:5:167:C:C2      | 48:5:269:G:C2      | 3.08                     | 0.41              |
| 48:5:1264:C:C4     | 48:5:1265:G:N7     | 2.88                     | 0.41              |
| 51:9:1398:G:C6     | 51:9:1399:C:C4     | 3.08                     | 0.41              |
| 56:EE:126:VAL:HG23 | 56:EE:156:MET:HA   | 2.02                     | 0.41              |
| 48:5:1736:A:C2     | 48:5:1794:A:C4     | 3.07                     | 0.41              |
| 48:5:208:A:N6      | 48:5:233:U:C4      | 2.88                     | 0.41              |
| 48:5:1416:G:C6     | 48:5:1417:C:C4     | 3.08                     | 0.41              |
| 48:5:2465:C:H2'    | 48:5:2466:G:O4'    | 2.20                     | 0.41              |
| 51:9:194:C:C2      | 51:9:206:G:N2      | 2.88                     | 0.41              |
| 48:5:4713:G:C2     | 48:5:4714:C:C2     | 3.07                     | 0.41              |
| 48:5:1431:C:H2'    | 48:5:1432:G:O4'    | 2.20                     | 0.41              |
| 51:9:52:G:C2       | 51:9:53:C:C2       | 3.08                     | 0.41              |
| 68:QQ:42:ILE:N     | 68:QQ:42:ILE:HD12  | 2.35                     | 0.41              |
| 48:5:4276:G:N2     | 48:5:4333:C:C2     | 2.88                     | 0.41              |
| 48:5:4247:G:C2     | 48:5:4262:C:C2     | 3.08                     | 0.41              |
| 51:9:1485:U:H2'    | 51:9:1486:A:O4'    | 2.20                     | 0.41              |
| 48:5:973:G:N2      | 48:5:1282:G:HO2'   | 2.09                     | 0.41              |
| 48:5:1379:C:O2     | 48:5:1379:C:O4'    | 2.37                     | 0.41              |
| 9:I:49:CYS:SG      | 9:I:49:CYS:O       | 2.78                     | 0.41              |
| 48:5:747:A:C2      | 48:5:918:G:N1      | 2.88                     | 0.41              |
| 48:5:2052:G:C2     | 48:5:2053:C:C2     | 3.09                     | 0.41              |
| 48:5:2533:C:C2     | 48:5:2534:C:C5     | 3.08                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:4586:G:H5''  | 48:5:4586:G:C8    | 2.52                     | 0.41              |
| 60:II:165:GLN:O   | 60:II:169:GLY:N   | 2.44                     | 0.41              |
| 48:5:2463:G:C6    | 48:5:2464:C:N4    | 2.89                     | 0.41              |
| 1:A:107:MET:SD    | 1:A:113:VAL:CG1   | 3.09                     | 0.41              |
| 48:5:2771:G:C2    | 48:5:2772:C:C2    | 3.08                     | 0.41              |
| 50:8:128:C:C5     | 50:8:129:C:C5     | 3.08                     | 0.41              |
| 48:5:4904:G:C6    | 48:5:4905:C:C4    | 3.07                     | 0.41              |
| 51:9:47:G:N2      | 51:9:48:C:C2      | 2.88                     | 0.41              |
| 25:Z:36:ARG:CD    | 25:Z:74:VAL:HG11  | 2.50                     | 0.41              |
| 71:TT:6:VAL:HG22  | 71:TT:65:TYR:CE2  | 2.54                     | 0.41              |
| 3:C:354:ALA:O     | 3:C:358:LEU:HG    | 2.20                     | 0.41              |
| 48:5:1573:G:C6    | 48:5:1574:G:N1    | 2.89                     | 0.41              |
| 48:5:1612:G:N3    | 48:5:1612:G:C2'   | 2.83                     | 0.41              |
| 48:5:1484:G:N3    | 48:5:1484:G:C2'   | 2.82                     | 0.41              |
| 48:5:1484:G:N3    | 48:5:1484:G:H2'   | 2.34                     | 0.41              |
| 6:F:60:HIS:HA     | 48:5:944:A:C8     | 2.55                     | 0.41              |
| 50:8:46:G:N2      | 50:8:47:C:C2      | 2.88                     | 0.41              |
| 48:5:1615:C:H2'   | 48:5:1616:U:O4'   | 2.19                     | 0.41              |
| 55:DD:70:THR:HG22 | 55:DD:86:LEU:HD13 | 2.02                     | 0.41              |
| 51:9:1661:A:H2'   | 51:9:1662:U:O4'   | 2.20                     | 0.41              |
| 48:5:2468:U:C2    | 48:5:2469:C:C5    | 3.08                     | 0.41              |
| 47:3:6:G:C6       | 47:3:7:A:C5       | 3.08                     | 0.41              |
| 48:5:2083:C:H4'   | 48:5:2084:C:OP2   | 2.21                     | 0.41              |
| 48:5:284:G:C2     | 48:5:304:C:O2     | 2.73                     | 0.41              |
| 2:B:41:VAL:HG21   | 2:B:196:TRP:CG    | 2.55                     | 0.41              |
| 48:5:1412:G:C6    | 48:5:1413:C:C4    | 3.08                     | 0.41              |
| 48:5:385:A:C2     | 48:5:386:A:C5     | 3.08                     | 0.41              |
| 48:5:1098:G:C6    | 48:5:1099:C:C4    | 3.08                     | 0.41              |
| 67:PP:34:MET:CE   | 67:PP:42:ARG:HA   | 2.49                     | 0.41              |
| 50:8:60:G:N2      | 50:8:64:U:C2      | 2.87                     | 0.41              |
| 48:5:952:G:H2'    | 48:5:953:C:O4'    | 2.20                     | 0.41              |
| 48:5:1557:C:C2    | 48:5:1571:G:N2    | 2.88                     | 0.41              |
| 48:5:4326:G:C2    | 48:5:4327:C:C2    | 3.09                     | 0.41              |
| 48:5:2050:G:C2    | 48:5:2051:C:C2    | 3.08                     | 0.41              |
| 48:5:517:C:C2     | 48:5:645:G:N2     | 2.88                     | 0.41              |
| 48:5:931:C:C2'    | 48:5:932:A:O5'    | 2.68                     | 0.41              |
| 51:9:427:U:O4'    | 51:9:427:U:O2     | 2.37                     | 0.41              |
| 63:LL:15:THR:HG22 | 63:LL:15:THR:O    | 2.20                     | 0.41              |
| 5:E:174:PRO:O     | 5:E:177:LEU:N     | 2.50                     | 0.41              |
| 1:A:243:THR:HG21  | 48:5:3748:A:O4'   | 2.20                     | 0.41              |
| 1:A:227:ARG:NH2   | 48:5:3659:G:O2'   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:5:4131:G:C6    | 48:5:4132:C:C4    | 3.09                     | 0.41              |
| 51:9:1184:G:C6    | 51:9:1185:C:C4    | 3.08                     | 0.41              |
| 48:5:3769:C:H2'   | 48:5:3770:U:O4'   | 2.20                     | 0.41              |
| 51:9:664:A:O2'    | 51:9:670:A:N1     | 2.39                     | 0.41              |
| 48:5:1959:U:O2'   | 48:5:1960:A:P     | 2.78                     | 0.41              |
| 51:9:943:U:H2'    | 51:9:944:A:O4'    | 2.20                     | 0.41              |
| 5:E:90:LYS:N      | 5:E:91:PRO:HD3    | 2.35                     | 0.41              |
| 48:5:4901:G:C2    | 48:5:4921:C:C2    | 3.08                     | 0.41              |
| 48:5:4901:G:N1    | 48:5:4921:C:C4    | 2.88                     | 0.41              |
| 48:5:1268:G:O4'   | 48:5:2111:G:C5    | 2.73                     | 0.41              |
| 3:C:30:ALA:HB1    | 3:C:31:PRO:HD2    | 2.02                     | 0.41              |
| 51:9:1771:G:C2    | 51:9:1772:C:C4    | 3.09                     | 0.41              |
| 48:5:4305:G:H2'   | 48:5:4305:G:N3    | 2.35                     | 0.41              |
| 48:5:665:C:O2     | 48:5:665:C:C2'    | 2.69                     | 0.41              |
| 48:5:1234:G:H2'   | 48:5:1235:G:C8    | 2.55                     | 0.41              |
| 20:U:21:PHE:CD1   | 20:U:80:LYS:HG2   | 2.55                     | 0.41              |
| 51:9:1654:G:C2    | 51:9:1655:C:C2    | 3.08                     | 0.41              |
| 48:5:80:C:C2      | 48:5:104:G:N2     | 2.89                     | 0.41              |
| 49:7:27:G:C6      | 49:7:28:C:C4      | 3.08                     | 0.41              |
| 48:5:2322:G:C2    | 48:5:2323:C:C2    | 3.09                     | 0.41              |
| 51:9:828:G:C2     | 51:9:829:C:C2     | 3.07                     | 0.41              |
| 48:5:4139:G:C2    | 48:5:4140:C:C2    | 3.08                     | 0.41              |
| 48:5:2703:G:C6    | 48:5:2704:C:C4    | 3.08                     | 0.41              |
| 46:2:65:G:C2      | 46:2:66:C:C2      | 3.08                     | 0.41              |
| 66:OO:39:ASP:N    | 66:OO:69:SER:OG   | 2.53                     | 0.41              |
| 48:5:1466:G:C2    | 48:5:1467:C:C2    | 3.09                     | 0.41              |
| 10:J:15:LEU:HD21  | 10:J:157:ILE:HD13 | 2.02                     | 0.41              |
| 13:N:11:TRP:CE3   | 13:N:44:ARG:NH2   | 2.89                     | 0.41              |
| 51:9:1323:U:H2'   | 51:9:1324:G:O4'   | 2.20                     | 0.41              |
| 18:S:84:TYR:C     | 18:S:84:TYR:CD1   | 2.94                     | 0.41              |
| 48:5:4950:U:O2    | 48:5:4950:U:O4'   | 2.38                     | 0.41              |
| 48:5:1329:G:H3'   | 48:5:1329:G:C8    | 2.55                     | 0.41              |
| 3:C:229:LEU:N     | 3:C:229:LEU:HD22  | 2.35                     | 0.41              |
| 18:S:173:ASN:HA   | 48:5:4762:A:H2    | 1.85                     | 0.41              |
| 51:9:1718:G:C6    | 51:9:1814:G:C6    | 3.09                     | 0.41              |
| 51:9:1459:G:C6    | 51:9:1460:C:C4    | 3.09                     | 0.41              |
| 14:O:15:LEU:HD11  | 14:O:129:LEU:HD13 | 2.01                     | 0.41              |
| 59:HH:105:THR:OG1 | 59:HH:108:SER:N   | 2.52                     | 0.41              |
| 48:5:972:C:H2'    | 48:5:973:G:H8     | 1.84                     | 0.41              |
| 48:5:4283:G:C6    | 48:5:4284:C:N4    | 2.88                     | 0.41              |
| 10:J:119:TYR:HB3  | 70:SS:12:ILE:HG21 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:5:4966:A:N1     | 48:5:4967:A:C6     | 2.88                     | 0.41              |
| 48:5:2478:C:N4     | 48:5:2479:G:O6     | 2.54                     | 0.41              |
| 12:M:34:ASN:ND2    | 48:5:1925:G:OP1    | 2.53                     | 0.41              |
| 51:9:1217:A:H2'    | 51:9:1218:C:C6     | 2.56                     | 0.41              |
| 48:5:4182:G:H5''   | 48:5:4183:G:OP2    | 2.20                     | 0.41              |
| 48:5:4492:U:O2'    | 48:5:4512:U:O2     | 2.22                     | 0.41              |
| 48:5:2889:G:C2     | 48:5:2890:C:C2     | 3.09                     | 0.41              |
| 51:9:978:G:C2      | 51:9:979:C:C2      | 3.09                     | 0.41              |
| 48:5:4131:G:C2     | 48:5:4132:C:C2     | 3.09                     | 0.41              |
| 51:9:1134:G:C2     | 51:9:1135:C:C2     | 3.08                     | 0.41              |
| 13:N:198:LEU:HD23  | 13:N:198:LEU:HA    | 1.94                     | 0.41              |
| 52:AA:147:LEU:HD12 | 52:AA:163:CYS:SG   | 2.60                     | 0.41              |
| 48:5:2273:G:C2     | 48:5:2274:C:C2     | 3.08                     | 0.41              |
| 48:5:1203:G:C2     | 48:5:1204:C:C2     | 3.08                     | 0.41              |
| 48:5:1275:G:C2     | 48:5:1276:C:C2     | 3.08                     | 0.41              |
| 48:5:1381:U:H5'    | 48:5:1382:G:OP2    | 2.21                     | 0.41              |
| 9:I:49:CYS:HB2     | 9:I:172:GLY:O      | 2.21                     | 0.41              |
| 51:9:1859:A:C2     | 51:9:1860:A:N1     | 2.88                     | 0.41              |
| 48:5:2547:G:C2     | 48:5:2548:C:C2     | 3.09                     | 0.41              |
| 51:9:832:G:C2      | 51:9:843:C:N3      | 2.89                     | 0.41              |
| 51:9:1551:U:C5     | 51:9:1577:G:C6     | 3.09                     | 0.41              |
| 48:5:1075:G:C6     | 48:5:1076:C:N4     | 2.88                     | 0.41              |
| 48:5:2052:G:C6     | 48:5:2053:C:C4     | 3.08                     | 0.41              |
| 48:5:127:G:C6      | 48:5:128:C:C4      | 3.08                     | 0.41              |
| 48:5:4664:A:H2'    | 48:5:4665:A:O4'    | 2.21                     | 0.41              |
| 51:9:49:C:N3       | 51:9:478:G:C6      | 2.88                     | 0.41              |
| 51:9:958:G:H2'     | 51:9:959:G:O4'     | 2.20                     | 0.41              |
| 4:D:43:LYS:O       | 4:D:46:THR:HG22    | 2.20                     | 0.41              |
| 48:5:751:G:N2      | 48:5:752:G:C5      | 2.89                     | 0.41              |
| 48:5:4395:U:H6     | 48:5:4395:U:H5'    | 1.85                     | 0.41              |
| 48:5:1422:G:C2     | 48:5:1464:C:C2     | 3.09                     | 0.41              |
| 60:II:60:LEU:HD23  | 60:II:185:ALA:HB2  | 2.03                     | 0.41              |
| 68:QQ:32:ILE:HD11  | 68:QQ:63:PHE:CD2   | 2.55                     | 0.41              |
| 51:9:1624:U:O4'    | 51:9:1624:U:O2     | 2.38                     | 0.41              |
| 51:9:921:G:C5      | 74:WW:28:ARG:HD2   | 2.56                     | 0.41              |
| 51:9:1275:G:HO2'   | 51:9:1276:A:P      | 2.43                     | 0.41              |
| 48:5:1424:G:H2'    | 48:5:1425:G:O4'    | 2.21                     | 0.41              |
| 60:II:102:VAL:HG11 | 60:II:175:ILE:HD11 | 2.01                     | 0.41              |
| 68:QQ:13:PHE:HA    | 68:QQ:22:VAL:HA    | 2.02                     | 0.41              |
| 48:5:169:G:C2      | 48:5:170:C:C2      | 3.09                     | 0.41              |
| 51:9:1384:C:O2'    | 51:9:1385:G:H5'    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:36:ASP:OD2     | 2:B:39:LYS:CE      | 2.62                     | 0.41              |
| 51:9:1130:G:N2     | 51:9:1131:G:C8     | 2.88                     | 0.41              |
| 74:WW:3:ARG:HE     | 74:WW:29:PRO:HG3   | 1.85                     | 0.41              |
| 51:9:1233:G:C2     | 51:9:1234:C:C2     | 3.08                     | 0.41              |
| 51:9:1233:G:H2'    | 51:9:1234:C:H5'    | 2.02                     | 0.41              |
| 56:EE:54:TYR:OH    | 56:EE:95:THR:HG21  | 2.21                     | 0.41              |
| 48:5:1205:G:N1     | 48:5:1206:C:C4     | 2.89                     | 0.41              |
| 51:9:1220:A:C6     | 51:9:1221:G:C5     | 3.08                     | 0.41              |
| 51:9:1537:A:C2     | 51:9:1538:C:C2     | 3.09                     | 0.41              |
| 48:5:2311:C:C2     | 48:5:2328:G:N2     | 2.89                     | 0.41              |
| 48:5:3937:C:H2'    | 48:5:3938:G:N2     | 2.35                     | 0.41              |
| 48:5:209:U:C4      | 48:5:233:U:O4      | 2.74                     | 0.41              |
| 8:H:5:LEU:HD13     | 8:H:60:TRP:CD2     | 2.56                     | 0.41              |
| 2:B:238:LYS:CE     | 48:5:3842:C:OP1    | 2.68                     | 0.41              |
| 48:5:4181:U:O4     | 48:5:4182:G:C6     | 2.73                     | 0.41              |
| 51:9:827:A:C5      | 51:9:828:G:C8      | 3.09                     | 0.41              |
| 48:5:2613:C:N4     | 48:5:2614:C:N4     | 2.68                     | 0.41              |
| 48:5:258:G:C6      | 48:5:259:C:C4      | 3.08                     | 0.41              |
| 52:AA:161:ILE:HG22 | 52:AA:163:CYS:SG   | 2.60                     | 0.41              |
| 48:5:368:C:C2      | 48:5:374:G:C2      | 3.09                     | 0.41              |
| 51:9:95:G:C6       | 51:9:96:C:C4       | 3.09                     | 0.41              |
| 48:5:307:A:N3      | 48:5:310:G:O2'     | 2.41                     | 0.41              |
| 48:5:119:G:H5''    | 48:5:119:G:C8      | 2.56                     | 0.41              |
| 48:5:2267:U:O4'    | 48:5:2267:U:O2     | 2.39                     | 0.41              |
| 15:P:10:ASN:N      | 15:P:10:ASN:OD1    | 2.53                     | 0.41              |
| 54:CC:116:THR:OG1  | 54:CC:118:ALA:O    | 2.38                     | 0.41              |
| 48:5:116:G:C2      | 48:5:117:C:C2      | 3.08                     | 0.41              |
| 50:8:49:G:C6       | 50:8:50:C:C4       | 3.09                     | 0.41              |
| 56:EE:234:PRO:CG   | 56:EE:238:LEU:HD11 | 2.51                     | 0.41              |
| 53:BB:171:ILE:HG21 | 53:BB:197:ILE:HG13 | 2.03                     | 0.41              |
| 51:9:1473:G:N2     | 51:9:1475:G:OP2    | 2.51                     | 0.41              |
| 48:5:1279:A:C4     | 48:5:1280:C:N3     | 2.89                     | 0.41              |
| 46:2:40:C:H4'      | 47:3:36:U:H1'      | 2.03                     | 0.41              |
| 51:9:65:C:O5'      | 58:GG:174:PRO:HA   | 2.21                     | 0.41              |
| 65:NN:87:ASP:OD2   | 65:NN:125:LEU:HD11 | 2.21                     | 0.41              |
| 48:5:730:G:N2      | 48:5:939:G:N2      | 2.69                     | 0.41              |
| 48:5:941:C:H2'     | 48:5:942:G:O4'     | 2.21                     | 0.41              |
| 48:5:1912:G:C6     | 48:5:1913:C:N4     | 2.89                     | 0.41              |
| 51:9:211:G:C2      | 51:9:212:C:C2      | 3.09                     | 0.41              |
| 48:5:2058:G:C6     | 48:5:2059:C:C4     | 3.09                     | 0.41              |
| 48:5:4473:A:C2     | 48:5:4474:A:C4     | 3.09                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 46:2:7:G:C2      | 46:2:49:C:C2       | 3.09                     | 0.41              |
| 48:5:1090:G:C6   | 48:5:1091:C:C4     | 3.08                     | 0.41              |
| 75:XX:82:THR:O   | 75:XX:118:VAL:HG13 | 2.21                     | 0.41              |
| 48:5:258:G:N2    | 48:5:259:C:C2      | 2.89                     | 0.41              |
| 48:5:4269:G:C6   | 48:5:4270:C:C4     | 3.09                     | 0.41              |
| 48:5:2645:G:C2   | 48:5:2646:C:C2     | 3.08                     | 0.41              |
| 52:AA:132:GLN:N  | 52:AA:133:PRO:HD2  | 2.36                     | 0.41              |
| 51:9:1611:G:OP2  | 70:SS:121:ARG:NH1  | 2.48                     | 0.41              |
| 51:9:1798:C:H2'  | 51:9:1799:G:O4'    | 2.21                     | 0.41              |
| 48:5:1439:C:O2   | 48:5:1439:C:O4'    | 2.39                     | 0.41              |
| 48:5:2625:U:C4   | 48:5:2626:U:C4     | 3.09                     | 0.41              |
| 51:9:1540:G:C2   | 51:9:1594:A:C2     | 3.09                     | 0.41              |
| 51:9:688:U:OP2   | 59:HH:122:LEU:N    | 2.54                     | 0.41              |
| 48:5:1969:G:HO2' | 48:5:1970:A:H5'    | 1.84                     | 0.41              |
| 48:5:971:U:C2'   | 48:5:972:C:H5'     | 2.51                     | 0.41              |
| 9:I:184:MET:HB3  | 9:I:184:MET:HE2    | 1.78                     | 0.41              |
| 51:9:1839:U:C6   | 51:9:1862:G:N2     | 2.88                     | 0.41              |
| 51:9:1835:A:C8   | 51:9:1863:A:N7     | 2.89                     | 0.41              |
| 48:5:2268:A:C4'  | 48:5:2269:C:H5'    | 2.49                     | 0.41              |
| 51:9:832:G:C2    | 51:9:833:C:C2      | 3.09                     | 0.41              |
| 3:C:76:ILE:HG22  | 3:C:77:PRO:CD      | 2.51                     | 0.41              |
| 51:9:1576:G:H2'  | 51:9:1577:G:O4'    | 2.20                     | 0.41              |
| 48:5:937:U:C2'   | 48:5:937:U:O2      | 2.69                     | 0.41              |
| 2:B:116:ARG:HB3  | 2:B:177:LYS:HA     | 2.03                     | 0.41              |
| 25:Z:28:ASN:C    | 25:Z:29:ILE:HD12   | 2.41                     | 0.41              |
| 48:5:93:G:C2'    | 48:5:94:A:C8       | 3.04                     | 0.41              |
| 48:5:44:A:O2'    | 48:5:94:A:N1       | 2.42                     | 0.41              |
| 17:R:58:HIS:HA   | 48:5:4646:U:OP1    | 2.21                     | 0.41              |
| 51:9:49:C:C2     | 51:9:478:G:N1      | 2.89                     | 0.41              |
| 51:9:378:U:H2'   | 51:9:379:C:O4'     | 2.21                     | 0.41              |
| 51:9:67:C:O2'    | 58:GG:165:GLU:OE1  | 2.39                     | 0.41              |
| 51:9:100:U:H2'   | 51:9:101:U:O4'     | 2.21                     | 0.41              |
| 67:PP:118:GLU:O  | 70:SS:120:HIS:N    | 2.53                     | 0.41              |
| 48:5:5031:G:C2   | 48:5:5032:C:C2     | 3.09                     | 0.41              |
| 48:5:1412:G:C2   | 48:5:1413:C:C2     | 3.09                     | 0.41              |
| 48:5:2517:A:N1   | 48:5:2518:G:C2     | 2.89                     | 0.41              |
| 48:5:369:G:N2    | 48:5:372:A:OP2     | 2.50                     | 0.41              |
| 6:F:168:ARG:HD2  | 6:F:211:TRP:CD1    | 2.55                     | 0.41              |
| 48:5:3786:U:O4'  | 48:5:4537:C:O2'    | 2.36                     | 0.41              |
| 46:2:29:C:H2'    | 46:2:30:G:O4'      | 2.21                     | 0.41              |
| 51:9:1293:A:H2'  | 51:9:1294:G:O4'    | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:9:1298:G:O2'    | 51:9:1299:A:O5'    | 2.38                     | 0.41              |
| 48:5:254:G:C6      | 48:5:255:C:C4      | 3.09                     | 0.41              |
| 48:5:2862:G:H2'    | 48:5:3619:G:O6     | 2.21                     | 0.41              |
| 21:V:26:ILE:HG22   | 21:V:101:ASN:HB3   | 2.03                     | 0.41              |
| 62:KK:62:PHE:CZ    | 62:KK:65:ARG:HA    | 2.56                     | 0.41              |
| 48:5:1721:G:C2     | 48:5:1722:C:C2     | 3.09                     | 0.41              |
| 48:5:4595:G:C2     | 48:5:4596:C:C2     | 3.08                     | 0.41              |
| 51:9:1184:G:C2     | 51:9:1185:C:C2     | 3.09                     | 0.41              |
| 66:OO:99:ALA:HB2   | 66:OO:108:PRO:HA   | 2.02                     | 0.41              |
| 74:WW:104:LEU:HB3  | 74:WW:125:ILE:HA   | 2.02                     | 0.41              |
| 3:C:266:THR:HG22   | 3:C:269:LYS:HB3    | 2.02                     | 0.41              |
| 51:9:856:C:O2      | 51:9:856:C:H2'     | 2.19                     | 0.41              |
| 9:I:35:ASP:N       | 9:I:35:ASP:OD1     | 2.54                     | 0.41              |
| 76:YY:62:THR:HA    | 76:YY:69:THR:HA    | 2.03                     | 0.41              |
| 16:Q:41:SER:OG     | 16:Q:44:ASN:ND2    | 2.54                     | 0.41              |
| 69:RR:126:MET:O    | 69:RR:127:ASN:ND2  | 2.54                     | 0.41              |
| 70:SS:25:LYS:HA    | 70:SS:55:ARG:HA    | 2.03                     | 0.41              |
| 48:5:4486:C:H2'    | 48:5:4487:A:O4'    | 2.21                     | 0.41              |
| 59:HH:40:LEU:O     | 59:HH:40:LEU:HD23  | 2.21                     | 0.41              |
| 48:5:3752:C:O2'    | 48:5:3753:G:P      | 2.78                     | 0.41              |
| 48:5:1970:A:C2     | 48:5:2016:C:C5     | 3.09                     | 0.41              |
| 9:I:187:GLU:O      | 9:I:188:LYS:HB2    | 2.21                     | 0.41              |
| 48:5:3723:A:C2     | 48:5:3730:U:N3     | 2.89                     | 0.41              |
| 51:9:1212:G:N2     | 51:9:1213:C:C2     | 2.89                     | 0.41              |
| 57:FF:127:ARG:HG3  | 57:FF:127:ARG:HH11 | 1.86                     | 0.41              |
| 50:8:154:G:C6      | 50:8:155:C:C4      | 3.09                     | 0.41              |
| 48:5:715:G:H1      | 48:5:953:C:H42     | 1.68                     | 0.41              |
| 17:R:5:ARG:NH2     | 48:5:2385:U:OP1    | 2.53                     | 0.41              |
| 18:S:84:TYR:HD1    | 18:S:84:TYR:C      | 2.25                     | 0.41              |
| 51:9:1275:G:O2'    | 51:9:1276:A:P      | 2.80                     | 0.41              |
| 59:HH:122:LEU:HD21 | 59:HH:126:HIS:CE1  | 2.56                     | 0.41              |
| 73:VV:9:VAL:HG13   | 73:VV:10:ASP:N     | 2.36                     | 0.41              |
| 48:5:4201:G:C6     | 48:5:4202:U:C4     | 3.09                     | 0.41              |
| 4:D:278:ASP:O      | 4:D:281:ALA:HB3    | 2.20                     | 0.41              |
| 25:Z:123:LYS:O     | 25:Z:124:THR:HG23  | 2.20                     | 0.41              |
| 48:5:960:A:N6      | 48:5:1283:G:O6     | 2.54                     | 0.41              |
| 48:5:1506:G:C2     | 48:5:1507:C:C2     | 3.09                     | 0.41              |
| 51:9:821:G:C6      | 61:JJ:147:PHE:CZ   | 3.08                     | 0.41              |
| 48:5:709:C:H2'     | 48:5:710:G:O4'     | 2.20                     | 0.41              |
| 3:C:228:THR:OG1    | 3:C:248:ARG:NH2    | 2.54                     | 0.41              |
| 48:5:1538:U:O2'    | 48:5:1629:G:OP1    | 2.33                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 48:5:4433:G:C2   | 48:5:4434:C:C2   | 3.09                     | 0.41              |
| 51:9:1137:U:N3   | 51:9:1148:A:C6   | 2.89                     | 0.40              |
| 47:3:68:C:N3     | 47:3:69:G:C5     | 2.89                     | 0.40              |
| 47:3:5:G:C2      | 47:3:6:G:C5      | 3.09                     | 0.40              |
| 48:5:4277:G:C2   | 48:5:4278:C:C2   | 3.09                     | 0.40              |
| 51:9:1236:G:C6   | 51:9:1237:C:C4   | 3.09                     | 0.40              |
| 48:5:1563:A:C8   | 51:9:678:U:C4'   | 2.98                     | 0.40              |
| 50:8:112:G:C6    | 50:8:113:C:C4    | 3.09                     | 0.40              |
| 48:5:1550:G:N1   | 48:5:1551:C:C2   | 2.89                     | 0.40              |
| 48:5:1633:G:H5'  | 48:5:1634:A:OP1  | 2.20                     | 0.40              |
| 6:F:94:VAL:HG13  | 6:F:142:ILE:HD12 | 2.04                     | 0.40              |
| 48:5:205:C:C2    | 48:5:211:G:C2    | 3.09                     | 0.40              |
| 48:5:2463:G:C6   | 48:5:2464:C:C4   | 3.10                     | 0.40              |
| 48:5:2457:G:C2   | 48:5:2458:C:C2   | 3.10                     | 0.40              |
| 46:2:30:G:C2     | 46:2:31:C:C2     | 3.09                     | 0.40              |
| 48:5:1466:G:C6   | 48:5:1467:C:C4   | 3.09                     | 0.40              |
| 51:9:999:G:C6    | 51:9:1000:C:C4   | 3.09                     | 0.40              |
| 51:9:95:G:C2     | 51:9:96:C:C2     | 3.09                     | 0.40              |
| 51:9:86:C:C4     | 51:9:87:U:C5     | 3.08                     | 0.40              |
| 1:A:117:GLU:OE1  | 1:A:121:GLY:N    | 2.52                     | 0.40              |
| 18:S:54:MET:HE3  | 18:S:54:MET:HB2  | 1.92                     | 0.40              |
| 3:C:293:LEU:HD22 | 16:Q:34:PHE:CD2  | 2.56                     | 0.40              |
| 4:D:20:PHE:CD1   | 49:7:10:C:C4     | 3.10                     | 0.40              |
| 48:5:247:G:C2    | 48:5:248:C:C2    | 3.09                     | 0.40              |
| 48:5:1441:C:N4   | 48:5:1442:C:N4   | 2.68                     | 0.40              |
| 48:5:1176:C:HO2' | 48:5:1177:U:C4'  | 2.29                     | 0.40              |
| 48:5:4530:U:H2'  | 48:5:4531:U:C6   | 2.55                     | 0.40              |
| 47:3:29:A:HO2'   | 47:3:30:G:C5'    | 2.23                     | 0.40              |
| 48:5:22:G:C2     | 50:8:35:C:C4     | 3.09                     | 0.40              |
| 51:9:164:A:H2'   | 51:9:165:G:C2    | 2.56                     | 0.40              |
| 51:9:834:C:N4    | 51:9:841:G:N1    | 2.69                     | 0.40              |
| 48:5:2481:G:N2   | 48:5:2498:C:C2   | 2.90                     | 0.40              |
| 51:9:1481:G:H2'  | 51:9:1482:C:O4'  | 2.21                     | 0.40              |
| 48:5:2726:G:C2   | 48:5:2727:C:C2   | 3.10                     | 0.40              |
| 51:9:45:A:N1     | 51:9:480:G:O2'   | 2.42                     | 0.40              |
| 1:A:200:ARG:NH1  | 48:5:3690:U:OP2  | 2.54                     | 0.40              |
| 48:5:35:U:H5'    | 48:5:36:U:OP2    | 2.21                     | 0.40              |
| 48:5:4714:C:C5   | 48:5:4715:C:C5   | 3.09                     | 0.40              |
| 51:9:1686:G:N2   | 51:9:1687:C:C2   | 2.90                     | 0.40              |
| 25:Z:38:TYR:CD1  | 25:Z:76:ASN:OD1  | 2.74                     | 0.40              |
| 3:C:195:LYS:NZ   | 50:8:21:C:OP1    | 2.52                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:27:VAL:HG11    | 3:C:128:LEU:HD13   | 2.03                     | 0.40              |
| 48:5:1932:A:H2'    | 48:5:1933:G:C8     | 2.57                     | 0.40              |
| 52:AA:157:VAL:HG23 | 52:AA:157:VAL:O    | 2.22                     | 0.40              |
| 48:5:4876:U:O4'    | 48:5:4876:U:O2     | 2.39                     | 0.40              |
| 48:5:1834:U:H2'    | 48:5:1834:U:O2     | 2.20                     | 0.40              |
| 53:BB:87:ILE:O     | 53:BB:98:THR:HA    | 2.21                     | 0.40              |
| 49:7:51:G:C2       | 49:7:52:C:C2       | 3.09                     | 0.40              |
| 48:5:695:G:H3'     | 48:5:696:C:H5'     | 2.02                     | 0.40              |
| 48:5:3832:U:H2'    | 48:5:3833:C:C6     | 2.57                     | 0.40              |
| 25:Z:95:VAL:HG12   | 25:Z:110:ALA:HA    | 2.03                     | 0.40              |
| 51:9:600:G:C8      | 51:9:631:U:C6      | 3.09                     | 0.40              |
| 76:YY:55:ILE:HG12  | 76:YY:75:ILE:HG23  | 2.02                     | 0.40              |
| 51:9:371:A:OP2     | 60:II:10:LYS:HB2   | 2.21                     | 0.40              |
| 48:5:518:G:C6      | 48:5:519:C:C4      | 3.09                     | 0.40              |
| 54:CC:109:ILE:HD11 | 54:CC:151:ILE:HD11 | 2.03                     | 0.40              |
| 48:5:1359:G:C2'    | 48:5:1360:G:C8     | 3.04                     | 0.40              |
| 48:5:102:G:C2'     | 48:5:1381:U:O2'    | 2.68                     | 0.40              |
| 48:5:4453:C:H2'    | 48:5:4454:G:O4'    | 2.21                     | 0.40              |
| 49:7:66:G:C6       | 49:7:67:C:N3       | 2.89                     | 0.40              |
| 50:8:154:G:C2      | 50:8:155:C:C2      | 3.09                     | 0.40              |
| 48:5:933:G:N1      | 48:5:939:G:N2      | 2.69                     | 0.40              |
| 48:5:2301:G:C2     | 48:5:2302:C:C2     | 3.09                     | 0.40              |
| 48:5:1808:C:C2     | 48:5:1831:G:C2     | 3.09                     | 0.40              |
| 48:5:4868:G:H3'    | 48:5:4869:U:H5''   | 2.03                     | 0.40              |
| 74:WW:89:TRP:HE3   | 74:WW:93:LEU:HD22  | 1.85                     | 0.40              |
| 51:9:380:G:OP1     | 60:II:31:ARG:NE    | 2.43                     | 0.40              |
| 72:UU:69:PRO:O     | 72:UU:70:CYS:SG    | 2.80                     | 0.40              |
| 51:9:827:A:C4      | 51:9:828:G:C8      | 3.09                     | 0.40              |
| 48:5:3706:C:H2'    | 48:5:3707:U:O4'    | 2.22                     | 0.40              |
| 48:5:116:G:C6      | 48:5:117:C:C4      | 3.10                     | 0.40              |
| 1:A:27:ALA:O       | 1:A:128:ARG:NH2    | 2.54                     | 0.40              |
| 14:O:14:HIS:CD2    | 14:O:124:LEU:HD12  | 2.57                     | 0.40              |
| 6:F:118:GLN:HG3    | 16:Q:3:VAL:HG22    | 2.03                     | 0.40              |
| 1:A:66:PRO:HG2     | 1:A:67:TYR:CE2     | 2.57                     | 0.40              |
| 51:9:1709:G:C6     | 51:9:1710:C:C4     | 3.08                     | 0.40              |
| 48:5:4495:G:C2     | 48:5:4506:C:C2     | 3.09                     | 0.40              |
| 7:G:140:VAL:HG13   | 7:G:200:THR:OG1    | 2.21                     | 0.40              |
| 48:5:2628:U:C4     | 48:5:2629:C:C5     | 3.09                     | 0.40              |
| 48:5:1356:U:H1'    | 48:5:1505:C:H1'    | 2.03                     | 0.40              |
| 50:8:76:C:H2'      | 50:8:77:A:O4'      | 2.22                     | 0.40              |
| 48:5:4614:G:C2     | 48:5:4615:C:C2     | 3.10                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:M:116:LYS:HG2   | 14:O:196:LEU:CD2   | 2.35                     | 0.40              |
| 51:9:752:G:N2      | 51:9:790:C:C2      | 2.90                     | 0.40              |
| 51:9:751:G:N1      | 51:9:792:C:C4      | 2.90                     | 0.40              |
| 48:5:4900:C:O2'    | 48:5:4901:G:P      | 2.80                     | 0.40              |
| 48:5:303:C:H2'     | 48:5:304:C:O4'     | 2.21                     | 0.40              |
| 48:5:3680:U:C2'    | 48:5:3680:U:O2     | 2.69                     | 0.40              |
| 48:5:3918:G:C2     | 48:5:3919:C:C2     | 3.10                     | 0.40              |
| 48:5:1780:A:N6     | 48:5:1781:U:C4     | 2.90                     | 0.40              |
| 48:5:940:C:C4      | 48:5:941:C:C4      | 3.10                     | 0.40              |
| 10:J:53:ALA:HB2    | 10:J:68:ILE:CD1    | 2.51                     | 0.40              |
| 48:5:4966:A:C2     | 48:5:4967:A:C6     | 3.10                     | 0.40              |
| 51:9:636:C:C4      | 51:9:637:U:C4      | 3.10                     | 0.40              |
| 51:9:480:G:C6      | 51:9:481:C:C4      | 3.10                     | 0.40              |
| 48:5:4408:G:C2     | 48:5:4409:C:C2     | 3.08                     | 0.40              |
| 50:8:31:G:C6       | 50:8:32:C:C4       | 3.10                     | 0.40              |
| 51:9:999:G:N2      | 51:9:1000:C:C2     | 2.89                     | 0.40              |
| 25:Z:73:LYS:HG2    | 25:Z:75:TYR:CZ     | 2.56                     | 0.40              |
| 3:C:143:ARG:N      | 3:C:179:ASP:OD1    | 2.54                     | 0.40              |
| 48:5:4745:G:N2     | 48:5:4746:C:N4     | 2.69                     | 0.40              |
| 53:BB:126:ASP:N    | 53:BB:126:ASP:OD1  | 2.54                     | 0.40              |
| 61:JJ:102:ILE:HG22 | 61:JJ:103:GLU:N    | 2.36                     | 0.40              |
| 6:F:181:LEU:HD11   | 6:F:209:PHE:HB2    | 2.02                     | 0.40              |
| 70:SS:59:LEU:HD23  | 70:SS:64:VAL:HG12  | 2.03                     | 0.40              |
| 50:8:115:G:C6      | 50:8:116:C:C4      | 3.10                     | 0.40              |
| 51:9:1571:G:C2     | 51:9:1572:C:C2     | 3.09                     | 0.40              |
| 47:3:69:G:C2       | 47:3:70:G:C5       | 3.09                     | 0.40              |
| 10:J:165:TRP:CH2   | 10:J:170:TYR:HE2   | 2.39                     | 0.40              |
| 46:2:39:G:C2       | 46:2:40:C:C2       | 3.09                     | 0.40              |
| 51:9:1129:G:H2'    | 51:9:1130:G:C1'    | 2.52                     | 0.40              |
| 5:E:217:GLN:HE22   | 5:E:233:LYS:HD2    | 1.85                     | 0.40              |
| 51:9:309:G:C2      | 51:9:310:C:C2      | 3.09                     | 0.40              |
| 58:GG:102:VAL:CG1  | 58:GG:109:LEU:HD11 | 2.52                     | 0.40              |
| 51:9:475:C:H2'     | 51:9:476:A:O4'     | 2.21                     | 0.40              |
| 51:9:1398:G:C2     | 51:9:1399:C:C2     | 3.10                     | 0.40              |
| 6:F:147:PRO:HA     | 6:F:243:ASN:OD1    | 2.22                     | 0.40              |
| 51:9:55:U:H2'      | 51:9:55:U:O2       | 2.21                     | 0.40              |
| 59:HH:43:LEU:HD21  | 59:HH:71:SER:CB    | 2.51                     | 0.40              |
| 48:5:990:C:C4      | 48:5:991:C:C5      | 3.10                     | 0.40              |
| 1:A:193:ARG:HH12   | 48:5:3686:G:P      | 2.44                     | 0.40              |
| 7:G:58:PRO:CD      | 23:X:46:PHE:HD2    | 2.34                     | 0.40              |
| 48:5:3846:C:H4'    | 48:5:4667:C:O2     | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 48:5:3705:G:C2   | 48:5:3706:C:C2   | 3.09                     | 0.40              |
| 51:9:1097:G:C2   | 51:9:1098:C:C2   | 3.10                     | 0.40              |
| 6:F:164:ILE:HD12 | 6:F:169:ILE:HB   | 2.03                     | 0.40              |
| 5:E:174:PRO:O    | 5:E:176:SER:N    | 2.55                     | 0.40              |
| 51:9:592:C:O4'   | 51:9:592:C:O2    | 2.36                     | 0.40              |
| 22:W:9:SER:HA    | 22:W:52:THR:HG22 | 2.04                     | 0.40              |
| 51:9:463:C:H2'   | 51:9:465:A:C8    | 2.56                     | 0.40              |
| 50:8:103:A:C8    | 50:8:104:A:C8    | 3.09                     | 0.40              |
| 77:ZZ:98:LYS:O   | 77:ZZ:109:TYR:HA | 2.21                     | 0.40              |
| 13:N:64:ILE:HD11 | 13:N:102:ALA:HA  | 2.03                     | 0.40              |
| 24:Y:24:HIS:CE1  | 24:Y:25:ILE:HG13 | 2.57                     | 0.40              |
| 48:5:1354:A:N1   | 48:5:1385:G:O2'  | 2.45                     | 0.40              |
| 51:9:936:G:C2    | 51:9:1007:C:C2   | 3.09                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 1   | A     | 242/244 (99%)  | 209 (86%) | 28 (12%) | 5 (2%)   | 9           | 48 |
| 2   | B     | 392/394 (100%) | 345 (88%) | 42 (11%) | 5 (1%)   | 15          | 58 |
| 3   | C     | 360/362 (99%)  | 322 (89%) | 27 (8%)  | 11 (3%)  | 5           | 39 |
| 4   | D     | 290/292 (99%)  | 262 (90%) | 25 (9%)  | 3 (1%)   | 19          | 64 |
| 5   | E     | 232/248 (94%)  | 179 (77%) | 36 (16%) | 17 (7%)  | 1           | 15 |
| 6   | F     | 223/225 (99%)  | 204 (92%) | 17 (8%)  | 2 (1%)   | 21          | 67 |
| 7   | G     | 239/241 (99%)  | 203 (85%) | 31 (13%) | 5 (2%)   | 9           | 48 |
| 8   | H     | 188/190 (99%)  | 165 (88%) | 20 (11%) | 3 (2%)   | 12          | 53 |
| 9   | I     | 200/213 (94%)  | 181 (90%) | 15 (8%)  | 4 (2%)   | 9           | 49 |
| 10  | J     | 167/169 (99%)  | 147 (88%) | 13 (8%)  | 7 (4%)   | 3           | 31 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 11  | L     | 208/210 (99%) | 180 (86%) | 16 (8%)  | 12 (6%)  | 2           | 21  |
| 12  | M     | 136/138 (99%) | 123 (90%) | 12 (9%)  | 1 (1%)   | 26          | 71  |
| 13  | N     | 201/203 (99%) | 181 (90%) | 20 (10%) | 0        | 100         | 100 |
| 14  | O     | 197/199 (99%) | 184 (93%) | 12 (6%)  | 1 (0%)   | 34          | 77  |
| 15  | P     | 151/153 (99%) | 135 (89%) | 16 (11%) | 0        | 100         | 100 |
| 16  | Q     | 185/187 (99%) | 169 (91%) | 14 (8%)  | 2 (1%)   | 17          | 62  |
| 17  | R     | 178/180 (99%) | 166 (93%) | 9 (5%)   | 3 (2%)   | 11          | 52  |
| 18  | S     | 173/175 (99%) | 157 (91%) | 12 (7%)  | 4 (2%)   | 8           | 46  |
| 19  | T     | 157/159 (99%) | 139 (88%) | 15 (10%) | 3 (2%)   | 10          | 49  |
| 20  | U     | 97/99 (98%)   | 82 (84%)  | 11 (11%) | 4 (4%)   | 3           | 32  |
| 21  | V     | 129/131 (98%) | 115 (89%) | 13 (10%) | 1 (1%)   | 24          | 69  |
| 22  | W     | 61/63 (97%)   | 56 (92%)  | 4 (7%)   | 1 (2%)   | 12          | 53  |
| 23  | X     | 117/119 (98%) | 109 (93%) | 6 (5%)   | 2 (2%)   | 11          | 52  |
| 24  | Y     | 132/134 (98%) | 114 (86%) | 17 (13%) | 1 (1%)   | 24          | 69  |
| 25  | Z     | 133/135 (98%) | 113 (85%) | 13 (10%) | 7 (5%)   | 2           | 23  |
| 26  | a     | 145/147 (99%) | 122 (84%) | 19 (13%) | 4 (3%)   | 6           | 41  |
| 27  | b     | 73/75 (97%)   | 67 (92%)  | 5 (7%)   | 1 (1%)   | 14          | 56  |
| 28  | c     | 92/94 (98%)   | 89 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 29  | d     | 105/107 (98%) | 91 (87%)  | 13 (12%) | 1 (1%)   | 19          | 64  |
| 30  | e     | 126/128 (98%) | 115 (91%) | 6 (5%)   | 5 (4%)   | 4           | 32  |
| 31  | f     | 107/109 (98%) | 94 (88%)  | 8 (8%)   | 5 (5%)   | 3           | 28  |
| 32  | g     | 112/114 (98%) | 103 (92%) | 8 (7%)   | 1 (1%)   | 21          | 67  |
| 33  | h     | 120/122 (98%) | 107 (89%) | 9 (8%)   | 4 (3%)   | 5           | 37  |
| 34  | i     | 100/102 (98%) | 92 (92%)  | 6 (6%)   | 2 (2%)   | 9           | 49  |
| 35  | j     | 84/86 (98%)   | 70 (83%)  | 9 (11%)  | 5 (6%)   | 2           | 20  |
| 36  | k     | 67/69 (97%)   | 56 (84%)  | 7 (10%)  | 4 (6%)   | 2           | 20  |
| 37  | l     | 48/50 (96%)   | 40 (83%)  | 7 (15%)  | 1 (2%)   | 9           | 48  |
| 38  | m     | 50/52 (96%)   | 44 (88%)  | 6 (12%)  | 0        | 100         | 100 |
| 39  | n     | 21/23 (91%)   | 21 (100%) | 0        | 0        | 100         | 100 |
| 40  | o     | 102/104 (98%) | 92 (90%)  | 7 (7%)   | 3 (3%)   | 6           | 40  |
| 41  | p     | 89/91 (98%)   | 80 (90%)  | 8 (9%)   | 1 (1%)   | 17          | 62  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 42  | r     | 123/125 (98%) | 102 (83%) | 14 (11%) | 7 (6%)   | 2           | 22 |
| 43  | s     | 196/198 (99%) | 164 (84%) | 22 (11%) | 10 (5%)  | 2           | 25 |
| 44  | t     | 161/163 (99%) | 102 (63%) | 33 (20%) | 26 (16%) | 0           | 2  |
| 45  | 1     | 13/15 (87%)   | 11 (85%)  | 0        | 2 (15%)  | 0           | 3  |
| 52  | AA    | 206/208 (99%) | 173 (84%) | 23 (11%) | 10 (5%)  | 3           | 26 |
| 53  | BB    | 211/213 (99%) | 165 (78%) | 33 (16%) | 13 (6%)  | 2           | 19 |
| 54  | CC    | 216/218 (99%) | 184 (85%) | 26 (12%) | 6 (3%)   | 6           | 41 |
| 55  | DD    | 225/227 (99%) | 181 (80%) | 33 (15%) | 11 (5%)  | 3           | 26 |
| 56  | EE    | 260/262 (99%) | 200 (77%) | 42 (16%) | 18 (7%)  | 1           | 16 |
| 57  | FF    | 189/191 (99%) | 160 (85%) | 21 (11%) | 8 (4%)   | 3           | 31 |
| 58  | GG    | 235/237 (99%) | 198 (84%) | 31 (13%) | 6 (3%)   | 7           | 43 |
| 59  | HH    | 187/189 (99%) | 148 (79%) | 25 (13%) | 14 (8%)  | 1           | 14 |
| 60  | II    | 204/206 (99%) | 168 (82%) | 28 (14%) | 8 (4%)   | 4           | 33 |
| 61  | JJ    | 183/185 (99%) | 153 (84%) | 20 (11%) | 10 (6%)  | 2           | 23 |
| 62  | KK    | 96/98 (98%)   | 65 (68%)  | 21 (22%) | 10 (10%) | 1           | 8  |
| 63  | LL    | 150/152 (99%) | 125 (83%) | 19 (13%) | 6 (4%)   | 4           | 32 |
| 64  | MM    | 122/124 (98%) | 87 (71%)  | 28 (23%) | 7 (6%)   | 2           | 22 |
| 65  | NN    | 148/150 (99%) | 126 (85%) | 17 (12%) | 5 (3%)   | 5           | 37 |
| 66  | OO    | 134/136 (98%) | 99 (74%)  | 21 (16%) | 14 (10%) | 1           | 8  |
| 67  | PP    | 125/127 (98%) | 107 (86%) | 15 (12%) | 3 (2%)   | 7           | 45 |
| 68  | QQ    | 139/141 (99%) | 116 (84%) | 18 (13%) | 5 (4%)   | 4           | 35 |
| 69  | RR    | 127/129 (98%) | 106 (84%) | 15 (12%) | 6 (5%)   | 3           | 28 |
| 70  | SS    | 135/137 (98%) | 114 (84%) | 16 (12%) | 5 (4%)   | 4           | 35 |
| 71  | TT    | 139/141 (99%) | 126 (91%) | 10 (7%)  | 3 (2%)   | 8           | 47 |
| 72  | UU    | 102/104 (98%) | 87 (85%)  | 9 (9%)   | 6 (6%)   | 2           | 21 |
| 73  | VV    | 81/83 (98%)   | 67 (83%)  | 10 (12%) | 4 (5%)   | 3           | 26 |
| 74  | WW    | 127/129 (98%) | 106 (84%) | 16 (13%) | 5 (4%)   | 4           | 33 |
| 75  | XX    | 139/141 (99%) | 118 (85%) | 13 (9%)  | 8 (6%)   | 2           | 21 |
| 76  | YY    | 124/126 (98%) | 99 (80%)  | 17 (14%) | 8 (6%)   | 1           | 18 |
| 77  | ZZ    | 73/75 (97%)   | 59 (81%)  | 12 (16%) | 2 (3%)   | 6           | 42 |
| 78  | aa    | 96/98 (98%)   | 73 (76%)  | 13 (14%) | 10 (10%) | 1           | 8  |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 79  | bb    | 81/83 (98%)       | 61 (75%)    | 16 (20%)   | 4 (5%)   | 3           | 26 |
| 80  | cc    | 59/61 (97%)       | 47 (80%)    | 10 (17%)   | 2 (3%)   | 5           | 37 |
| 81  | dd    | 51/53 (96%)       | 45 (88%)    | 3 (6%)     | 3 (6%)   | 2           | 21 |
| 82  | ee    | 55/57 (96%)       | 40 (73%)    | 12 (22%)   | 3 (6%)   | 2           | 23 |
| 83  | ff    | 58/68 (85%)       | 50 (86%)    | 6 (10%)    | 2 (3%)   | 5           | 37 |
| 84  | gg    | 311/313 (99%)     | 269 (86%)   | 33 (11%)   | 9 (3%)   | 6           | 40 |
| 86  | ii    | 414/416 (100%)    | 380 (92%)   | 26 (6%)    | 8 (2%)   | 10          | 49 |
| 87  | jj    | 568/594 (96%)     | 513 (90%)   | 41 (7%)    | 14 (2%)  | 7           | 44 |
| All | All   | 12492/12709 (98%) | 10717 (86%) | 1333 (11%) | 442 (4%) | 8           | 36 |

All (442) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 196 | TRP  |
| 3   | C     | 273 | LEU  |
| 5   | E     | 91  | PRO  |
| 5   | E     | 95  | ASP  |
| 5   | E     | 118 | PRO  |
| 5   | E     | 175 | LEU  |
| 5   | E     | 221 | PRO  |
| 7   | G     | 45  | ILE  |
| 7   | G     | 128 | VAL  |
| 8   | H     | 40  | HIS  |
| 8   | H     | 110 | SER  |
| 9   | I     | 47  | PRO  |
| 11  | L     | 64  | VAL  |
| 11  | L     | 67  | HIS  |
| 17  | R     | 36  | ASN  |
| 18  | S     | 165 | PRO  |
| 20  | U     | 47  | ILE  |
| 25  | Z     | 84  | ARG  |
| 26  | a     | 90  | ALA  |
| 29  | d     | 94  | GLU  |
| 30  | e     | 92  | ASN  |
| 31  | f     | 80  | ASN  |
| 33  | h     | 7   | ARG  |
| 36  | k     | 61  | PRO  |
| 40  | o     | 32  | SER  |
| 42  | r     | 86  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | s     | 62  | ARG  |
| 43  | s     | 201 | PRO  |
| 44  | t     | 29  | ALA  |
| 44  | t     | 30  | PRO  |
| 44  | t     | 31  | LYS  |
| 44  | t     | 53  | TRP  |
| 44  | t     | 89  | PRO  |
| 44  | t     | 144 | ASP  |
| 44  | t     | 148 | PRO  |
| 44  | t     | 149 | HIS  |
| 52  | AA    | 186 | ARG  |
| 53  | BB    | 57  | ILE  |
| 53  | BB    | 179 | ASN  |
| 53  | BB    | 191 | ASP  |
| 55  | DD    | 192 | TRP  |
| 55  | DD    | 202 | LYS  |
| 55  | DD    | 223 | ILE  |
| 56  | EE    | 24  | THR  |
| 56  | EE    | 76  | VAL  |
| 56  | EE    | 118 | GLU  |
| 56  | EE    | 164 | LEU  |
| 56  | EE    | 196 | THR  |
| 57  | FF    | 34  | SER  |
| 57  | FF    | 163 | PHE  |
| 58  | GG    | 174 | PRO  |
| 59  | HH    | 18  | GLU  |
| 59  | HH    | 66  | VAL  |
| 59  | HH    | 116 | ARG  |
| 59  | HH    | 159 | ASP  |
| 60  | II    | 27  | TYR  |
| 60  | II    | 155 | ASN  |
| 60  | II    | 157 | LYS  |
| 61  | JJ    | 4   | ALA  |
| 61  | JJ    | 22  | LYS  |
| 61  | JJ    | 121 | LYS  |
| 62  | KK    | 95  | ARG  |
| 64  | MM    | 79  | VAL  |
| 64  | MM    | 102 | LYS  |
| 64  | MM    | 114 | TYR  |
| 65  | NN    | 24  | THR  |
| 66  | OO    | 56  | VAL  |
| 66  | OO    | 65  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 66  | OO    | 128 | ARG  |
| 66  | OO    | 140 | THR  |
| 68  | QQ    | 43  | GLU  |
| 68  | QQ    | 64  | ALA  |
| 69  | RR    | 88  | VAL  |
| 69  | RR    | 93  | GLN  |
| 71  | TT    | 34  | VAL  |
| 72  | UU    | 107 | GLU  |
| 73  | VV    | 41  | LYS  |
| 73  | VV    | 48  | GLY  |
| 75  | XX    | 34  | THR  |
| 75  | XX    | 42  | GLY  |
| 76  | YY    | 104 | ARG  |
| 76  | YY    | 114 | MET  |
| 76  | YY    | 120 | THR  |
| 77  | ZZ    | 113 | THR  |
| 78  | aa    | 10  | ARG  |
| 82  | ee    | 9   | VAL  |
| 84  | gg    | 254 | PRO  |
| 84  | gg    | 282 | GLU  |
| 86  | ii    | 298 | THR  |
| 87  | jj    | 245 | SER  |
| 87  | jj    | 455 | ILE  |
| 1   | A     | 217 | GLN  |
| 2   | B     | 38  | SER  |
| 2   | B     | 302 | ASN  |
| 3   | C     | 73  | VAL  |
| 3   | C     | 155 | GLU  |
| 3   | C     | 275 | SER  |
| 4   | D     | 187 | SER  |
| 5   | E     | 85  | LEU  |
| 5   | E     | 92  | VAL  |
| 5   | E     | 174 | PRO  |
| 5   | E     | 234 | GLU  |
| 10  | J     | 116 | GLY  |
| 10  | J     | 155 | HIS  |
| 11  | L     | 63  | THR  |
| 11  | L     | 143 | GLU  |
| 11  | L     | 172 | GLU  |
| 17  | R     | 130 | ASN  |
| 18  | S     | 88  | SER  |
| 19  | T     | 81  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | U     | 98  | ASP  |
| 23  | X     | 131 | ASP  |
| 25  | Z     | 34  | SER  |
| 26  | a     | 76  | ASP  |
| 30  | e     | 44  | ARG  |
| 34  | i     | 11  | LEU  |
| 35  | j     | 36  | LYS  |
| 35  | j     | 39  | TYR  |
| 36  | k     | 32  | VAL  |
| 42  | r     | 67  | ARG  |
| 42  | r     | 71  | ARG  |
| 43  | s     | 70  | GLU  |
| 43  | s     | 106 | LYS  |
| 43  | s     | 109 | ALA  |
| 44  | t     | 5   | PHE  |
| 44  | t     | 26  | SER  |
| 44  | t     | 39  | PRO  |
| 44  | t     | 58  | ILE  |
| 44  | t     | 106 | PHE  |
| 52  | AA    | 44  | ASP  |
| 52  | AA    | 45  | GLY  |
| 53  | BB    | 86  | LEU  |
| 53  | BB    | 140 | VAL  |
| 53  | BB    | 153 | THR  |
| 54  | CC    | 181 | PRO  |
| 54  | CC    | 190 | SER  |
| 55  | DD    | 219 | PRO  |
| 56  | EE    | 40  | GLU  |
| 56  | EE    | 95  | THR  |
| 56  | EE    | 153 | LEU  |
| 56  | EE    | 231 | GLY  |
| 57  | FF    | 33  | ILE  |
| 57  | FF    | 80  | GLY  |
| 58  | GG    | 152 | ASP  |
| 59  | HH    | 160 | LYS  |
| 59  | HH    | 190 | PRO  |
| 60  | II    | 138 | ASN  |
| 61  | JJ    | 21  | GLU  |
| 61  | JJ    | 120 | ALA  |
| 62  | KK    | 3   | MET  |
| 62  | KK    | 39  | ASN  |
| 62  | KK    | 63  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | LL    | 66  | VAL  |
| 63  | LL    | 135 | SER  |
| 64  | MM    | 15  | ASN  |
| 65  | NN    | 3   | ARG  |
| 65  | NN    | 28  | LEU  |
| 65  | NN    | 138 | ASN  |
| 66  | OO    | 39  | ASP  |
| 66  | OO    | 104 | ARG  |
| 66  | OO    | 129 | ILE  |
| 67  | PP    | 14  | LYS  |
| 67  | PP    | 75  | VAL  |
| 69  | RR    | 63  | ARG  |
| 70  | SS    | 12  | ILE  |
| 70  | SS    | 92  | ASP  |
| 71  | TT    | 29  | LYS  |
| 71  | TT    | 39  | LEU  |
| 72  | UU    | 50  | VAL  |
| 74  | WW    | 3   | ARG  |
| 75  | XX    | 10  | ALA  |
| 75  | XX    | 110 | HIS  |
| 76  | YY    | 84  | LYS  |
| 76  | YY    | 95  | GLY  |
| 76  | YY    | 127 | ALA  |
| 77  | ZZ    | 112 | ASN  |
| 78  | aa    | 8   | ASN  |
| 78  | aa    | 25  | ASN  |
| 79  | bb    | 4   | ALA  |
| 79  | bb    | 82  | LYS  |
| 80  | cc    | 26  | GLN  |
| 81  | dd    | 47  | ALA  |
| 82  | ee    | 43  | VAL  |
| 84  | gg    | 61  | GLY  |
| 84  | gg    | 161 | SER  |
| 86  | ii    | 31  | GLY  |
| 86  | ii    | 224 | LEU  |
| 86  | ii    | 315 | GLY  |
| 86  | ii    | 387 | ALA  |
| 2   | B     | 18  | PRO  |
| 3   | C     | 16  | GLU  |
| 3   | C     | 132 | ALA  |
| 3   | C     | 248 | ARG  |
| 5   | E     | 96  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 179 | ARG  |
| 5   | E     | 232 | GLU  |
| 6   | F     | 239 | GLU  |
| 9   | I     | 205 | PRO  |
| 10  | J     | 11  | PRO  |
| 10  | J     | 146 | ARG  |
| 16  | Q     | 14  | ARG  |
| 17  | R     | 19  | LYS  |
| 21  | V     | 14  | PHE  |
| 25  | Z     | 55  | ALA  |
| 25  | Z     | 124 | THR  |
| 26  | a     | 92  | LYS  |
| 30  | e     | 125 | PRO  |
| 30  | e     | 126 | ASN  |
| 31  | f     | 37  | ASP  |
| 31  | f     | 79  | GLY  |
| 33  | h     | 97  | LYS  |
| 34  | i     | 3   | LEU  |
| 37  | l     | 47  | THR  |
| 42  | r     | 19  | LYS  |
| 42  | r     | 85  | ASN  |
| 43  | s     | 69  | LEU  |
| 43  | s     | 108 | PRO  |
| 43  | s     | 142 | GLY  |
| 44  | t     | 54  | LYS  |
| 44  | t     | 67  | ARG  |
| 44  | t     | 105 | THR  |
| 44  | t     | 137 | GLN  |
| 52  | AA    | 50  | ASN  |
| 52  | AA    | 191 | ARG  |
| 53  | BB    | 88  | THR  |
| 53  | BB    | 206 | PRO  |
| 54  | CC    | 255 | LEU  |
| 55  | DD    | 175 | VAL  |
| 55  | DD    | 200 | PRO  |
| 55  | DD    | 222 | PRO  |
| 56  | EE    | 98  | ASN  |
| 57  | FF    | 119 | SER  |
| 58  | GG    | 59  | GLN  |
| 59  | HH    | 107 | LYS  |
| 60  | II    | 137 | LEU  |
| 60  | II    | 143 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | JJ    | 39  | ASN  |
| 62  | KK    | 31  | LYS  |
| 62  | KK    | 65  | ARG  |
| 62  | KK    | 92  | ALA  |
| 63  | LL    | 147 | LYS  |
| 63  | LL    | 149 | ALA  |
| 64  | MM    | 100 | PRO  |
| 66  | OO    | 32  | HIS  |
| 66  | OO    | 64  | ALA  |
| 67  | PP    | 15  | PHE  |
| 68  | QQ    | 100 | VAL  |
| 70  | SS    | 11  | HIS  |
| 73  | VV    | 21  | ASN  |
| 73  | VV    | 45  | ARG  |
| 74  | WW    | 93  | LEU  |
| 75  | XX    | 6   | GLY  |
| 76  | YY    | 34  | THR  |
| 78  | aa    | 9   | GLY  |
| 78  | aa    | 61  | ALA  |
| 78  | aa    | 62  | TYR  |
| 78  | aa    | 64  | LEU  |
| 78  | aa    | 65  | PRO  |
| 79  | bb    | 75  | GLU  |
| 86  | ii    | 28  | ARG  |
| 87  | jj    | 22  | ARG  |
| 87  | jj    | 179 | ALA  |
| 87  | jj    | 421 | THR  |
| 1   | A     | 180 | LEU  |
| 2   | B     | 54  | THR  |
| 5   | E     | 129 | PHE  |
| 5   | E     | 224 | GLN  |
| 8   | H     | 101 | ILE  |
| 11  | L     | 5   | ARG  |
| 11  | L     | 52  | SER  |
| 19  | T     | 29  | THR  |
| 24  | Y     | 83  | GLU  |
| 25  | Z     | 31  | ASP  |
| 26  | a     | 98  | ALA  |
| 30  | e     | 89  | LEU  |
| 32  | g     | 65  | MET  |
| 33  | h     | 89  | ARG  |
| 36  | k     | 29  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | p     | 41  | PHE  |
| 44  | t     | 2   | PRO  |
| 44  | t     | 18  | THR  |
| 45  | 1     | 57  | ARG  |
| 52  | AA    | 43  | SER  |
| 52  | AA    | 102 | ARG  |
| 52  | AA    | 207 | PRO  |
| 53  | BB    | 154 | SER  |
| 54  | CC    | 264 | SER  |
| 55  | DD    | 191 | PRO  |
| 56  | EE    | 30  | ARG  |
| 56  | EE    | 73  | ASP  |
| 57  | FF    | 132 | GLY  |
| 59  | HH    | 16  | PRO  |
| 59  | HH    | 100 | ILE  |
| 59  | HH    | 111 | LYS  |
| 59  | HH    | 119 | SER  |
| 59  | HH    | 122 | LEU  |
| 61  | JJ    | 138 | ARG  |
| 61  | JJ    | 147 | PHE  |
| 63  | LL    | 28  | THR  |
| 63  | LL    | 32  | LYS  |
| 66  | OO    | 138 | ASP  |
| 69  | RR    | 121 | GLN  |
| 70  | SS    | 7   | GLU  |
| 72  | UU    | 51  | LYS  |
| 72  | UU    | 105 | SER  |
| 72  | UU    | 118 | ASP  |
| 74  | WW    | 112 | ASP  |
| 75  | XX    | 53  | GLU  |
| 75  | XX    | 129 | SER  |
| 78  | aa    | 15  | ARG  |
| 78  | aa    | 35  | ALA  |
| 82  | ee    | 22  | GLN  |
| 83  | ff    | 85  | LYS  |
| 83  | ff    | 117 | PRO  |
| 84  | gg    | 12  | LYS  |
| 84  | gg    | 190 | GLY  |
| 84  | gg    | 205 | SER  |
| 84  | gg    | 296 | GLN  |
| 86  | ii    | 373 | PRO  |
| 86  | ii    | 386 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | jj    | 285 | PHE  |
| 1   | A     | 130 | SER  |
| 2   | B     | 309 | LEU  |
| 4   | D     | 20  | PHE  |
| 5   | E     | 218 | LEU  |
| 5   | E     | 229 | PHE  |
| 7   | G     | 123 | ALA  |
| 7   | G     | 125 | LYS  |
| 10  | J     | 153 | ALA  |
| 11  | L     | 6   | ASN  |
| 11  | L     | 103 | ARG  |
| 16  | Q     | 148 | VAL  |
| 20  | U     | 27  | HIS  |
| 25  | Z     | 91  | LEU  |
| 31  | f     | 107 | PRO  |
| 33  | h     | 40  | ALA  |
| 35  | j     | 34  | CYS  |
| 35  | j     | 61  | THR  |
| 36  | k     | 21  | LYS  |
| 40  | o     | 77  | CYS  |
| 42  | r     | 11  | ARG  |
| 43  | s     | 34  | ASN  |
| 44  | t     | 7   | PRO  |
| 45  | l     | 64  | PRO  |
| 52  | AA    | 6   | ASP  |
| 52  | AA    | 36  | GLN  |
| 53  | BB    | 22  | VAL  |
| 53  | BB    | 24  | PRO  |
| 53  | BB    | 208 | HIS  |
| 54  | CC    | 134 | ASN  |
| 55  | DD    | 4   | GLN  |
| 55  | DD    | 199 | GLY  |
| 56  | EE    | 109 | PHE  |
| 56  | EE    | 131 | VAL  |
| 56  | EE    | 152 | PRO  |
| 57  | FF    | 37  | ASP  |
| 57  | FF    | 79  | HIS  |
| 58  | GG    | 54  | GLY  |
| 58  | GG    | 105 | ASN  |
| 58  | GG    | 146 | ASN  |
| 59  | HH    | 6   | ALA  |
| 60  | II    | 131 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | KK    | 90  | VAL  |
| 64  | MM    | 103 | VAL  |
| 64  | MM    | 116 | LYS  |
| 66  | OO    | 54  | CYS  |
| 68  | QQ    | 35  | ASN  |
| 69  | RR    | 42  | PRO  |
| 69  | RR    | 95  | ILE  |
| 70  | SS    | 59  | LEU  |
| 74  | WW    | 66  | THR  |
| 79  | bb    | 38  | PRO  |
| 80  | cc    | 64  | GLU  |
| 81  | dd    | 11  | PRO  |
| 87  | jj    | 47  | ILE  |
| 1   | A     | 67  | TYR  |
| 3   | C     | 222 | ARG  |
| 3   | C     | 309 | ILE  |
| 10  | J     | 124 | GLY  |
| 11  | L     | 100 | PRO  |
| 11  | L     | 169 | ILE  |
| 14  | O     | 49  | ARG  |
| 18  | S     | 5   | GLY  |
| 20  | U     | 67  | LYS  |
| 22  | W     | 15  | PRO  |
| 31  | f     | 106 | TYR  |
| 35  | j     | 60  | GLY  |
| 40  | o     | 33  | LEU  |
| 44  | t     | 10  | ILE  |
| 44  | t     | 19  | GLY  |
| 44  | t     | 22  | VAL  |
| 54  | CC    | 261 | PHE  |
| 56  | EE    | 90  | ILE  |
| 59  | HH    | 57  | ARG  |
| 61  | JJ    | 102 | ILE  |
| 62  | KK    | 32  | HIS  |
| 62  | KK    | 43  | LEU  |
| 65  | NN    | 60  | VAL  |
| 66  | OO    | 24  | GLY  |
| 66  | OO    | 33  | ILE  |
| 66  | OO    | 38  | ASN  |
| 68  | QQ    | 32  | ILE  |
| 87  | jj    | 24  | GLU  |
| 87  | jj    | 45  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | jj    | 402 | GLY  |
| 3   | C     | 133 | LEU  |
| 9   | I     | 99  | ILE  |
| 27  | b     | 21  | ILE  |
| 43  | s     | 73  | PRO  |
| 76  | YY    | 126 | GLY  |
| 87  | jj    | 129 | PRO  |
| 4   | D     | 125 | VAL  |
| 9   | I     | 201 | PRO  |
| 11  | L     | 134 | PRO  |
| 25  | Z     | 90  | PRO  |
| 53  | BB    | 93  | GLY  |
| 55  | DD    | 218 | LEU  |
| 56  | EE    | 195 | ILE  |
| 60  | II    | 126 | GLY  |
| 61  | JJ    | 18  | ARG  |
| 87  | jj    | 249 | VAL  |
| 87  | jj    | 432 | ILE  |
| 3   | C     | 265 | GLY  |
| 5   | E     | 103 | VAL  |
| 6   | F     | 230 | VAL  |
| 7   | G     | 238 | GLY  |
| 19  | T     | 44  | GLY  |
| 75  | XX    | 116 | PRO  |
| 84  | gg    | 163 | PRO  |
| 87  | jj    | 263 | ILE  |
| 10  | J     | 174 | ILE  |
| 12  | M     | 7   | VAL  |
| 18  | S     | 155 | PRO  |
| 44  | t     | 3   | PRO  |
| 44  | t     | 98  | ILE  |
| 72  | UU    | 52  | GLY  |
| 74  | WW    | 29  | PRO  |
| 81  | dd    | 23  | VAL  |
| 23  | X     | 119 | ILE  |
| 42  | r     | 69  | GLY  |
| 44  | t     | 23  | GLY  |
| 56  | EE    | 107 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 187/187 (100%) | 161 (86%) | 26 (14%) | 4           | 23 |
| 2   | B     | 336/342 (98%)  | 291 (87%) | 45 (13%) | 5           | 25 |
| 3   | C     | 302/302 (100%) | 260 (86%) | 42 (14%) | 4           | 23 |
| 4   | D     | 247/247 (100%) | 218 (88%) | 29 (12%) | 7           | 30 |
| 5   | E     | 208/221 (94%)  | 185 (89%) | 23 (11%) | 8           | 34 |
| 6   | F     | 194/195 (100%) | 165 (85%) | 29 (15%) | 4           | 20 |
| 7   | G     | 206/206 (100%) | 182 (88%) | 24 (12%) | 7           | 30 |
| 8   | H     | 169/169 (100%) | 148 (88%) | 21 (12%) | 6           | 28 |
| 9   | I     | 174/180 (97%)  | 153 (88%) | 21 (12%) | 6           | 29 |
| 10  | J     | 142/142 (100%) | 126 (89%) | 16 (11%) | 7           | 32 |
| 11  | L     | 176/176 (100%) | 145 (82%) | 31 (18%) | 2           | 12 |
| 12  | M     | 117/117 (100%) | 102 (87%) | 15 (13%) | 5           | 27 |
| 13  | N     | 171/171 (100%) | 152 (89%) | 19 (11%) | 8           | 34 |
| 14  | O     | 171/171 (100%) | 144 (84%) | 27 (16%) | 3           | 18 |
| 15  | P     | 134/134 (100%) | 120 (90%) | 14 (10%) | 9           | 38 |
| 16  | Q     | 163/163 (100%) | 145 (89%) | 18 (11%) | 8           | 35 |
| 17  | R     | 159/159 (100%) | 140 (88%) | 19 (12%) | 6           | 29 |
| 18  | S     | 156/156 (100%) | 132 (85%) | 24 (15%) | 3           | 19 |
| 19  | T     | 139/139 (100%) | 122 (88%) | 17 (12%) | 6           | 28 |
| 20  | U     | 89/89 (100%)   | 82 (92%)  | 7 (8%)   | 15          | 52 |
| 21  | V     | 101/101 (100%) | 84 (83%)  | 17 (17%) | 2           | 14 |
| 22  | W     | 55/55 (100%)   | 50 (91%)  | 5 (9%)   | 12          | 45 |
| 23  | X     | 107/107 (100%) | 97 (91%)  | 10 (9%)  | 11          | 44 |
| 24  | Y     | 124/124 (100%) | 107 (86%) | 17 (14%) | 4           | 24 |
| 25  | Z     | 117/117 (100%) | 109 (93%) | 8 (7%)   | 20          | 59 |
| 26  | a     | 119/119 (100%) | 107 (90%) | 12 (10%) | 9           | 39 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 27  | b     | 62/62 (100%)   | 57 (92%)  | 5 (8%)   | 15          | 51 |
| 28  | c     | 79/79 (100%)   | 66 (84%)  | 13 (16%) | 3           | 15 |
| 29  | d     | 98/98 (100%)   | 82 (84%)  | 16 (16%) | 3           | 16 |
| 30  | e     | 114/114 (100%) | 99 (87%)  | 15 (13%) | 5           | 26 |
| 31  | f     | 88/88 (100%)   | 76 (86%)  | 12 (14%) | 5           | 24 |
| 32  | g     | 98/98 (100%)   | 83 (85%)  | 15 (15%) | 3           | 19 |
| 33  | h     | 109/109 (100%) | 97 (89%)  | 12 (11%) | 8           | 35 |
| 34  | i     | 86/86 (100%)   | 81 (94%)  | 5 (6%)   | 25          | 65 |
| 35  | j     | 73/73 (100%)   | 62 (85%)  | 11 (15%) | 3           | 20 |
| 36  | k     | 64/64 (100%)   | 56 (88%)  | 8 (12%)  | 6           | 28 |
| 37  | l     | 47/47 (100%)   | 40 (85%)  | 7 (15%)  | 4           | 20 |
| 38  | m     | 48/48 (100%)   | 39 (81%)  | 9 (19%)  | 2           | 9  |
| 39  | n     | 22/22 (100%)   | 18 (82%)  | 4 (18%)  | 2           | 11 |
| 40  | o     | 92/92 (100%)   | 79 (86%)  | 13 (14%) | 4           | 22 |
| 41  | p     | 74/74 (100%)   | 68 (92%)  | 6 (8%)   | 15          | 51 |
| 42  | r     | 109/109 (100%) | 88 (81%)  | 21 (19%) | 2           | 8  |
| 43  | s     | 166/166 (100%) | 155 (93%) | 11 (7%)  | 21          | 61 |
| 44  | t     | 136/136 (100%) | 128 (94%) | 8 (6%)   | 24          | 64 |
| 45  | 1     | 13/13 (100%)   | 12 (92%)  | 1 (8%)   | 16          | 53 |
| 52  | AA    | 174/174 (100%) | 152 (87%) | 22 (13%) | 5           | 27 |
| 53  | BB    | 194/194 (100%) | 169 (87%) | 25 (13%) | 5           | 26 |
| 54  | CC    | 183/183 (100%) | 155 (85%) | 28 (15%) | 3           | 19 |
| 55  | DD    | 190/190 (100%) | 168 (88%) | 22 (12%) | 7           | 31 |
| 56  | EE    | 223/223 (100%) | 183 (82%) | 40 (18%) | 2           | 11 |
| 57  | FF    | 161/161 (100%) | 126 (78%) | 35 (22%) | 1           | 6  |
| 58  | GG    | 207/207 (100%) | 179 (86%) | 28 (14%) | 5           | 25 |
| 59  | HH    | 169/169 (100%) | 151 (89%) | 18 (11%) | 8           | 36 |
| 60  | II    | 178/178 (100%) | 155 (87%) | 23 (13%) | 5           | 26 |
| 61  | JJ    | 161/161 (100%) | 141 (88%) | 20 (12%) | 6           | 28 |
| 62  | KK    | 89/89 (100%)   | 76 (85%)  | 13 (15%) | 4           | 21 |
| 63  | LL    | 136/136 (100%) | 110 (81%) | 26 (19%) | 2           | 9  |

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| Mol | Chain | Analysed           | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|--------------------|------------|------------|-------------|----|
| 64  | MM    | 104/104 (100%)     | 85 (82%)   | 19 (18%)   | 2           | 10 |
| 65  | NN    | 130/130 (100%)     | 108 (83%)  | 22 (17%)   | 2           | 14 |
| 66  | OO    | 106/106 (100%)     | 81 (76%)   | 25 (24%)   | 1           | 4  |
| 67  | PP    | 116/116 (100%)     | 98 (84%)   | 18 (16%)   | 3           | 18 |
| 68  | QQ    | 117/117 (100%)     | 102 (87%)  | 15 (13%)   | 5           | 27 |
| 69  | RR    | 117/117 (100%)     | 102 (87%)  | 15 (13%)   | 5           | 27 |
| 70  | SS    | 119/119 (100%)     | 100 (84%)  | 19 (16%)   | 3           | 17 |
| 71  | TT    | 112/112 (100%)     | 94 (84%)   | 18 (16%)   | 3           | 17 |
| 72  | UU    | 94/94 (100%)       | 79 (84%)   | 15 (16%)   | 3           | 17 |
| 73  | VV    | 67/67 (100%)       | 61 (91%)   | 6 (9%)     | 12          | 46 |
| 74  | WW    | 112/112 (100%)     | 99 (88%)   | 13 (12%)   | 7           | 31 |
| 75  | XX    | 113/113 (100%)     | 94 (83%)   | 19 (17%)   | 2           | 14 |
| 76  | YY    | 108/108 (100%)     | 88 (82%)   | 20 (18%)   | 2           | 10 |
| 77  | ZZ    | 66/66 (100%)       | 59 (89%)   | 7 (11%)    | 8           | 37 |
| 78  | aa    | 85/85 (100%)       | 77 (91%)   | 8 (9%)     | 11          | 43 |
| 79  | bb    | 75/75 (100%)       | 62 (83%)   | 13 (17%)   | 2           | 13 |
| 80  | cc    | 54/54 (100%)       | 44 (82%)   | 10 (18%)   | 2           | 10 |
| 81  | dd    | 47/47 (100%)       | 40 (85%)   | 7 (15%)    | 4           | 20 |
| 82  | ee    | 47/47 (100%)       | 39 (83%)   | 8 (17%)    | 2           | 14 |
| 83  | ff    | 58/61 (95%)        | 57 (98%)   | 1 (2%)     | 68          | 89 |
| 84  | gg    | 272/272 (100%)     | 250 (92%)  | 22 (8%)    | 15          | 51 |
| 86  | ii    | 358/358 (100%)     | 324 (90%)  | 34 (10%)   | 11          | 42 |
| 87  | jj    | 506/522 (97%)      | 487 (96%)  | 19 (4%)    | 40          | 76 |
| All | All   | 10889/10934 (100%) | 9508 (87%) | 1381 (13%) | 10          | 27 |

All (1381) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | ILE  |
| 1   | A     | 44  | ILE  |
| 1   | A     | 49  | ILE  |
| 1   | A     | 64  | ARG  |
| 1   | A     | 82  | ILE  |
| 1   | A     | 96  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 97  | ASN  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 125 | LYS  |
| 1   | A     | 128 | ARG  |
| 1   | A     | 142 | GLU  |
| 1   | A     | 158 | ILE  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 175 | ILE  |
| 1   | A     | 180 | LEU  |
| 1   | A     | 193 | ARG  |
| 1   | A     | 194 | ASN  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 207 | VAL  |
| 1   | A     | 218 | HIS  |
| 1   | A     | 221 | LYS  |
| 1   | A     | 226 | ARG  |
| 1   | A     | 227 | ARG  |
| 1   | A     | 233 | ARG  |
| 1   | A     | 235 | VAL  |
| 1   | A     | 242 | ARG  |
| 2   | B     | 4   | ARG  |
| 2   | B     | 10  | ARG  |
| 2   | B     | 17  | LEU  |
| 2   | B     | 19  | ARG  |
| 2   | B     | 21  | ARG  |
| 2   | B     | 31  | SER  |
| 2   | B     | 43  | LEU  |
| 2   | B     | 56  | ILE  |
| 2   | B     | 61  | ASP  |
| 2   | B     | 62  | ARG  |
| 2   | B     | 66  | LYS  |
| 2   | B     | 67  | VAL  |
| 2   | B     | 90  | VAL  |
| 2   | B     | 97  | ARG  |
| 2   | B     | 99  | LEU  |
| 2   | B     | 101 | THR  |
| 2   | B     | 103 | LYS  |
| 2   | B     | 115 | LYS  |
| 2   | B     | 116 | ARG  |
| 2   | B     | 135 | LYS  |
| 2   | B     | 138 | GLN  |
| 2   | B     | 146 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 162 | VAL  |
| 2   | B     | 167 | GLN  |
| 2   | B     | 173 | LEU  |
| 2   | B     | 203 | GLN  |
| 2   | B     | 213 | GLN  |
| 2   | B     | 214 | ASP  |
| 2   | B     | 228 | TYR  |
| 2   | B     | 244 | THR  |
| 2   | B     | 248 | LEU  |
| 2   | B     | 258 | HIS  |
| 2   | B     | 261 | ARG  |
| 2   | B     | 262 | VAL  |
| 2   | B     | 309 | LEU  |
| 2   | B     | 314 | ILE  |
| 2   | B     | 329 | ASP  |
| 2   | B     | 333 | LEU  |
| 2   | B     | 340 | THR  |
| 2   | B     | 352 | LEU  |
| 2   | B     | 356 | LYS  |
| 2   | B     | 357 | ARG  |
| 2   | B     | 366 | LYS  |
| 2   | B     | 381 | THR  |
| 2   | B     | 383 | GLU  |
| 3   | C     | 14  | LYS  |
| 3   | C     | 20  | LYS  |
| 3   | C     | 44  | LEU  |
| 3   | C     | 54  | VAL  |
| 3   | C     | 55  | SER  |
| 3   | C     | 57  | LEU  |
| 3   | C     | 66  | SER  |
| 3   | C     | 71  | ARG  |
| 3   | C     | 80  | ARG  |
| 3   | C     | 95  | MET  |
| 3   | C     | 101 | MET  |
| 3   | C     | 113 | ARG  |
| 3   | C     | 114 | ARG  |
| 3   | C     | 122 | TYR  |
| 3   | C     | 124 | ILE  |
| 3   | C     | 144 | ILE  |
| 3   | C     | 147 | VAL  |
| 3   | C     | 150 | LEU  |
| 3   | C     | 155 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 159 | GLU  |
| 3   | C     | 165 | LYS  |
| 3   | C     | 175 | LYS  |
| 3   | C     | 179 | ASP  |
| 3   | C     | 188 | ARG  |
| 3   | C     | 193 | LYS  |
| 3   | C     | 204 | ARG  |
| 3   | C     | 208 | CYS  |
| 3   | C     | 222 | ARG  |
| 3   | C     | 232 | VAL  |
| 3   | C     | 237 | ILE  |
| 3   | C     | 246 | VAL  |
| 3   | C     | 267 | TRP  |
| 3   | C     | 281 | MET  |
| 3   | C     | 284 | MET  |
| 3   | C     | 287 | THR  |
| 3   | C     | 294 | LYS  |
| 3   | C     | 307 | LYS  |
| 3   | C     | 312 | ARG  |
| 3   | C     | 333 | LYS  |
| 3   | C     | 342 | ARG  |
| 3   | C     | 345 | ARG  |
| 3   | C     | 348 | LYS  |
| 4   | D     | 4   | VAL  |
| 4   | D     | 22  | ARG  |
| 4   | D     | 33  | ARG  |
| 4   | D     | 37  | VAL  |
| 4   | D     | 50  | ARG  |
| 4   | D     | 66  | TYR  |
| 4   | D     | 89  | LYS  |
| 4   | D     | 94  | ASN  |
| 4   | D     | 104 | LEU  |
| 4   | D     | 110 | LEU  |
| 4   | D     | 111 | ASN  |
| 4   | D     | 124 | GLU  |
| 4   | D     | 128 | ASP  |
| 4   | D     | 152 | ARG  |
| 4   | D     | 179 | ARG  |
| 4   | D     | 189 | GLU  |
| 4   | D     | 196 | ARG  |
| 4   | D     | 202 | GLN  |
| 4   | D     | 206 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 208 | MET  |
| 4   | D     | 225 | GLN  |
| 4   | D     | 234 | ASP  |
| 4   | D     | 248 | ARG  |
| 4   | D     | 249 | GLU  |
| 4   | D     | 256 | LYS  |
| 4   | D     | 264 | LYS  |
| 4   | D     | 268 | ARG  |
| 4   | D     | 279 | ARG  |
| 4   | D     | 293 | ARG  |
| 5   | E     | 43  | ASN  |
| 5   | E     | 46  | LEU  |
| 5   | E     | 52  | ARG  |
| 5   | E     | 55  | ARG  |
| 5   | E     | 58  | MET  |
| 5   | E     | 101 | ARG  |
| 5   | E     | 105 | LEU  |
| 5   | E     | 126 | ARG  |
| 5   | E     | 134 | ARG  |
| 5   | E     | 136 | LEU  |
| 5   | E     | 137 | ARG  |
| 5   | E     | 148 | ILE  |
| 5   | E     | 162 | LYS  |
| 5   | E     | 190 | VAL  |
| 5   | E     | 197 | ILE  |
| 5   | E     | 206 | LYS  |
| 5   | E     | 212 | TYR  |
| 5   | E     | 230 | ASP  |
| 5   | E     | 233 | LYS  |
| 5   | E     | 250 | ASP  |
| 5   | E     | 254 | LEU  |
| 5   | E     | 282 | LEU  |
| 5   | E     | 284 | PHE  |
| 6   | F     | 33  | LYS  |
| 6   | F     | 41  | GLN  |
| 6   | F     | 44  | LEU  |
| 6   | F     | 49  | ARG  |
| 6   | F     | 68  | ARG  |
| 6   | F     | 70  | GLU  |
| 6   | F     | 72  | ARG  |
| 6   | F     | 76  | MET  |
| 6   | F     | 82  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 90  | LYS  |
| 6   | F     | 91  | LEU  |
| 6   | F     | 100 | ILE  |
| 6   | F     | 101 | ASN  |
| 6   | F     | 127 | LEU  |
| 6   | F     | 137 | ILE  |
| 6   | F     | 154 | GLU  |
| 6   | F     | 179 | ARG  |
| 6   | F     | 181 | LEU  |
| 6   | F     | 189 | MET  |
| 6   | F     | 190 | GLU  |
| 6   | F     | 192 | LEU  |
| 6   | F     | 201 | LYS  |
| 6   | F     | 202 | ARG  |
| 6   | F     | 214 | LYS  |
| 6   | F     | 216 | SER  |
| 6   | F     | 234 | ASP  |
| 6   | F     | 239 | GLU  |
| 6   | F     | 248 | ARG  |
| 6   | F     | 249 | MET  |
| 7   | G     | 28  | VAL  |
| 7   | G     | 73  | ARG  |
| 7   | G     | 75  | LYS  |
| 7   | G     | 81  | ASN  |
| 7   | G     | 90  | GLN  |
| 7   | G     | 95  | LEU  |
| 7   | G     | 106 | THR  |
| 7   | G     | 110 | LYS  |
| 7   | G     | 112 | GLN  |
| 7   | G     | 131 | LYS  |
| 7   | G     | 148 | GLU  |
| 7   | G     | 150 | LYS  |
| 7   | G     | 151 | LYS  |
| 7   | G     | 154 | LEU  |
| 7   | G     | 170 | LEU  |
| 7   | G     | 173 | LEU  |
| 7   | G     | 175 | ARG  |
| 7   | G     | 177 | MET  |
| 7   | G     | 189 | ARG  |
| 7   | G     | 202 | VAL  |
| 7   | G     | 210 | GLU  |
| 7   | G     | 217 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 220 | GLU  |
| 7   | G     | 240 | ASN  |
| 8   | H     | 1   | MET  |
| 8   | H     | 20  | LEU  |
| 8   | H     | 26  | ILE  |
| 8   | H     | 28  | LYS  |
| 8   | H     | 41  | ILE  |
| 8   | H     | 52  | LYS  |
| 8   | H     | 54  | ARG  |
| 8   | H     | 57  | VAL  |
| 8   | H     | 59  | LYS  |
| 8   | H     | 66  | GLU  |
| 8   | H     | 74  | CYS  |
| 8   | H     | 78  | GLN  |
| 8   | H     | 98  | HIS  |
| 8   | H     | 111 | LEU  |
| 8   | H     | 125 | ARG  |
| 8   | H     | 128 | MET  |
| 8   | H     | 129 | ARG  |
| 8   | H     | 162 | GLN  |
| 8   | H     | 173 | ARG  |
| 8   | H     | 177 | ASP  |
| 8   | H     | 183 | GLU  |
| 9   | I     | 13  | LYS  |
| 9   | I     | 35  | ASP  |
| 9   | I     | 36  | LEU  |
| 9   | I     | 39  | LYS  |
| 9   | I     | 43  | VAL  |
| 9   | I     | 48  | LEU  |
| 9   | I     | 76  | MET  |
| 9   | I     | 88  | ARG  |
| 9   | I     | 116 | ARG  |
| 9   | I     | 136 | MET  |
| 9   | I     | 139 | ARG  |
| 9   | I     | 144 | ASN  |
| 9   | I     | 153 | ARG  |
| 9   | I     | 163 | GLN  |
| 9   | I     | 164 | LYS  |
| 9   | I     | 180 | GLU  |
| 9   | I     | 195 | CYS  |
| 9   | I     | 198 | LYS  |
| 9   | I     | 202 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 208 | LYS  |
| 9   | I     | 212 | LEU  |
| 10  | J     | 15  | LEU  |
| 10  | J     | 16  | ARG  |
| 10  | J     | 33  | LEU  |
| 10  | J     | 34  | THR  |
| 10  | J     | 49  | VAL  |
| 10  | J     | 55  | TYR  |
| 10  | J     | 72  | CYS  |
| 10  | J     | 90  | ARG  |
| 10  | J     | 91  | GLU  |
| 10  | J     | 110 | GLN  |
| 10  | J     | 111 | GLU  |
| 10  | J     | 113 | ILE  |
| 10  | J     | 146 | ARG  |
| 10  | J     | 151 | ILE  |
| 10  | J     | 167 | GLN  |
| 10  | J     | 168 | GLN  |
| 11  | L     | 10  | LEU  |
| 11  | L     | 28  | GLN  |
| 11  | L     | 35  | ARG  |
| 11  | L     | 49  | ARG  |
| 11  | L     | 59  | VAL  |
| 11  | L     | 61  | CYS  |
| 11  | L     | 64  | VAL  |
| 11  | L     | 67  | HIS  |
| 11  | L     | 74  | ARG  |
| 11  | L     | 77  | SER  |
| 11  | L     | 92  | ARG  |
| 11  | L     | 94  | ILE  |
| 11  | L     | 99  | ASP  |
| 11  | L     | 107 | THR  |
| 11  | L     | 111 | GLN  |
| 11  | L     | 113 | ASN  |
| 11  | L     | 115 | GLN  |
| 11  | L     | 121 | ARG  |
| 11  | L     | 123 | LYS  |
| 11  | L     | 129 | ARG  |
| 11  | L     | 130 | LYS  |
| 11  | L     | 143 | GLU  |
| 11  | L     | 145 | LYS  |
| 11  | L     | 158 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | L     | 162 | LYS  |
| 11  | L     | 165 | LYS  |
| 11  | L     | 186 | ARG  |
| 11  | L     | 190 | ARG  |
| 11  | L     | 195 | ARG  |
| 11  | L     | 198 | ARG  |
| 11  | L     | 201 | GLU  |
| 12  | M     | 5   | ARG  |
| 12  | M     | 8   | GLU  |
| 12  | M     | 25  | VAL  |
| 12  | M     | 33  | GLN  |
| 12  | M     | 38  | VAL  |
| 12  | M     | 48  | GLN  |
| 12  | M     | 53  | LYS  |
| 12  | M     | 57  | LEU  |
| 12  | M     | 61  | ILE  |
| 12  | M     | 70  | GLN  |
| 12  | M     | 96  | GLU  |
| 12  | M     | 105 | THR  |
| 12  | M     | 118 | MET  |
| 12  | M     | 119 | ARG  |
| 12  | M     | 130 | LEU  |
| 13  | N     | 9   | GLU  |
| 13  | N     | 17  | ASP  |
| 13  | N     | 26  | ARG  |
| 13  | N     | 32  | GLN  |
| 13  | N     | 61  | ILE  |
| 13  | N     | 64  | ILE  |
| 13  | N     | 72  | LYS  |
| 13  | N     | 77  | LYS  |
| 13  | N     | 80  | THR  |
| 13  | N     | 87  | HIS  |
| 13  | N     | 89  | VAL  |
| 13  | N     | 104 | GLU  |
| 13  | N     | 108 | ARG  |
| 13  | N     | 136 | ASP  |
| 13  | N     | 147 | ASP  |
| 13  | N     | 174 | LEU  |
| 13  | N     | 197 | THR  |
| 13  | N     | 199 | GLN  |
| 13  | N     | 202 | ARG  |
| 14  | O     | 5   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | O     | 18  | ARG  |
| 14  | O     | 31  | ARG  |
| 14  | O     | 36  | VAL  |
| 14  | O     | 37  | ARG  |
| 14  | O     | 38  | CYS  |
| 14  | O     | 42  | ASN  |
| 14  | O     | 49  | ARG  |
| 14  | O     | 60  | LYS  |
| 14  | O     | 61  | ARG  |
| 14  | O     | 62  | MET  |
| 14  | O     | 67  | SER  |
| 14  | O     | 74  | ARG  |
| 14  | O     | 82  | ARG  |
| 14  | O     | 85  | ARG  |
| 14  | O     | 103 | LYS  |
| 14  | O     | 117 | ARG  |
| 14  | O     | 128 | ARG  |
| 14  | O     | 130 | LYS  |
| 14  | O     | 145 | VAL  |
| 14  | O     | 165 | LYS  |
| 14  | O     | 175 | MET  |
| 14  | O     | 179 | LYS  |
| 14  | O     | 187 | LYS  |
| 14  | O     | 195 | VAL  |
| 14  | O     | 201 | PHE  |
| 14  | O     | 202 | LEU  |
| 15  | P     | 5   | SER  |
| 15  | P     | 7   | ASP  |
| 15  | P     | 25  | HIS  |
| 15  | P     | 57  | CYS  |
| 15  | P     | 69  | ARG  |
| 15  | P     | 86  | LYS  |
| 15  | P     | 91  | LEU  |
| 15  | P     | 92  | LEU  |
| 15  | P     | 99  | GLU  |
| 15  | P     | 100 | SER  |
| 15  | P     | 105 | LYS  |
| 15  | P     | 127 | ARG  |
| 15  | P     | 128 | ARG  |
| 15  | P     | 147 | GLU  |
| 16  | Q     | 13  | VAL  |
| 16  | Q     | 31  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | Q     | 37  | ARG  |
| 16  | Q     | 54  | SER  |
| 16  | Q     | 63  | LEU  |
| 16  | Q     | 75  | ARG  |
| 16  | Q     | 78  | LYS  |
| 16  | Q     | 85  | THR  |
| 16  | Q     | 89  | ASP  |
| 16  | Q     | 91  | ARG  |
| 16  | Q     | 93  | GLN  |
| 16  | Q     | 95  | VAL  |
| 16  | Q     | 97  | LYS  |
| 16  | Q     | 108 | ARG  |
| 16  | Q     | 112 | ARG  |
| 16  | Q     | 140 | SER  |
| 16  | Q     | 143 | ARG  |
| 16  | Q     | 187 | LYS  |
| 17  | R     | 10  | LEU  |
| 17  | R     | 15  | LEU  |
| 17  | R     | 39  | GLN  |
| 17  | R     | 40  | GLN  |
| 17  | R     | 43  | LYS  |
| 17  | R     | 50  | ILE  |
| 17  | R     | 52  | ARG  |
| 17  | R     | 75  | HIS  |
| 17  | R     | 89  | MET  |
| 17  | R     | 98  | ARG  |
| 17  | R     | 99  | MET  |
| 17  | R     | 106 | LEU  |
| 17  | R     | 107 | ARG  |
| 17  | R     | 113 | LYS  |
| 17  | R     | 117 | ARG  |
| 17  | R     | 123 | LEU  |
| 17  | R     | 133 | LYS  |
| 17  | R     | 138 | LEU  |
| 17  | R     | 178 | GLN  |
| 18  | S     | 2   | LYS  |
| 18  | S     | 8   | ARG  |
| 18  | S     | 9   | GLU  |
| 18  | S     | 17  | LEU  |
| 18  | S     | 39  | VAL  |
| 18  | S     | 43  | ARG  |
| 18  | S     | 67  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | S     | 70  | LYS  |
| 18  | S     | 82  | LEU  |
| 18  | S     | 83  | ARG  |
| 18  | S     | 84  | TYR  |
| 18  | S     | 86  | SER  |
| 18  | S     | 91  | HIS  |
| 18  | S     | 95  | ARG  |
| 18  | S     | 98  | ARG  |
| 18  | S     | 100 | LEU  |
| 18  | S     | 102 | THR  |
| 18  | S     | 125 | GLN  |
| 18  | S     | 127 | MET  |
| 18  | S     | 132 | ILE  |
| 18  | S     | 147 | ASP  |
| 18  | S     | 149 | LYS  |
| 18  | S     | 156 | HIS  |
| 18  | S     | 159 | LEU  |
| 19  | T     | 5   | LYS  |
| 19  | T     | 9   | ARG  |
| 19  | T     | 17  | ARG  |
| 19  | T     | 33  | ILE  |
| 19  | T     | 41  | ASP  |
| 19  | T     | 52  | MET  |
| 19  | T     | 60  | LYS  |
| 19  | T     | 81  | LYS  |
| 19  | T     | 96  | ILE  |
| 19  | T     | 99  | SER  |
| 19  | T     | 117 | LYS  |
| 19  | T     | 118 | GLU  |
| 19  | T     | 131 | GLN  |
| 19  | T     | 142 | ARG  |
| 19  | T     | 144 | ASN  |
| 19  | T     | 157 | GLU  |
| 19  | T     | 159 | MET  |
| 20  | U     | 33  | ILE  |
| 20  | U     | 46  | ARG  |
| 20  | U     | 65  | ARG  |
| 20  | U     | 67  | LYS  |
| 20  | U     | 80  | LYS  |
| 20  | U     | 97  | ARG  |
| 20  | U     | 99  | TRP  |
| 21  | V     | 15  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | V     | 18  | LEU  |
| 21  | V     | 31  | ASN  |
| 21  | V     | 35  | LYS  |
| 21  | V     | 46  | LYS  |
| 21  | V     | 51  | ARG  |
| 21  | V     | 57  | VAL  |
| 21  | V     | 60  | MET  |
| 21  | V     | 61  | VAL  |
| 21  | V     | 82  | ILE  |
| 21  | V     | 91  | LYS  |
| 21  | V     | 97  | TYR  |
| 21  | V     | 99  | GLU  |
| 21  | V     | 106 | VAL  |
| 21  | V     | 109 | LYS  |
| 21  | V     | 113 | LYS  |
| 21  | V     | 123 | LYS  |
| 22  | W     | 4   | GLU  |
| 22  | W     | 27  | LYS  |
| 22  | W     | 41  | LEU  |
| 22  | W     | 43  | LYS  |
| 22  | W     | 57  | ARG  |
| 23  | X     | 39  | LYS  |
| 23  | X     | 41  | ARG  |
| 23  | X     | 50  | LYS  |
| 23  | X     | 52  | LEU  |
| 23  | X     | 59  | LYS  |
| 23  | X     | 94  | ASN  |
| 23  | X     | 111 | GLN  |
| 23  | X     | 129 | ARG  |
| 23  | X     | 145 | ASP  |
| 23  | X     | 152 | LYS  |
| 24  | Y     | 2   | LYS  |
| 24  | Y     | 7   | VAL  |
| 24  | Y     | 8   | THR  |
| 24  | Y     | 28  | LYS  |
| 24  | Y     | 34  | LEU  |
| 24  | Y     | 50  | ARG  |
| 24  | Y     | 52  | ASP  |
| 24  | Y     | 55  | VAL  |
| 24  | Y     | 59  | ARG  |
| 24  | Y     | 65  | GLN  |
| 24  | Y     | 72  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | Y     | 74  | TYR  |
| 24  | Y     | 79  | VAL  |
| 24  | Y     | 87  | ARG  |
| 24  | Y     | 104 | VAL  |
| 24  | Y     | 115 | ARG  |
| 24  | Y     | 126 | ARG  |
| 25  | Z     | 11  | VAL  |
| 25  | Z     | 17  | ARG  |
| 25  | Z     | 57  | MET  |
| 25  | Z     | 59  | LYS  |
| 25  | Z     | 67  | LYS  |
| 25  | Z     | 93  | LYS  |
| 25  | Z     | 108 | ARG  |
| 25  | Z     | 112 | ARG  |
| 26  | a     | 10  | LYS  |
| 26  | a     | 12  | ARG  |
| 26  | a     | 39  | HIS  |
| 26  | a     | 40  | HIS  |
| 26  | a     | 46  | ASP  |
| 26  | a     | 47  | LYS  |
| 26  | a     | 52  | TYR  |
| 26  | a     | 59  | ARG  |
| 26  | a     | 63  | LEU  |
| 26  | a     | 84  | GLU  |
| 26  | a     | 122 | VAL  |
| 26  | a     | 132 | ARG  |
| 27  | b     | 22  | LYS  |
| 27  | b     | 28  | ARG  |
| 27  | b     | 39  | PHE  |
| 27  | b     | 43  | MET  |
| 27  | b     | 51  | LYS  |
| 28  | c     | 28  | VAL  |
| 28  | c     | 37  | MET  |
| 28  | c     | 40  | GLN  |
| 28  | c     | 50  | ASN  |
| 28  | c     | 59  | GLU  |
| 28  | c     | 61  | GLU  |
| 28  | c     | 77  | ASN  |
| 28  | c     | 78  | ASN  |
| 28  | c     | 81  | LEU  |
| 28  | c     | 87  | LYS  |
| 28  | c     | 91  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | c     | 94  | LEU  |
| 28  | c     | 98  | ASP  |
| 29  | d     | 19  | GLU  |
| 29  | d     | 23  | ARG  |
| 29  | d     | 26  | THR  |
| 29  | d     | 31  | LYS  |
| 29  | d     | 36  | VAL  |
| 29  | d     | 44  | ARG  |
| 29  | d     | 48  | GLU  |
| 29  | d     | 75  | LYS  |
| 29  | d     | 78  | ARG  |
| 29  | d     | 79  | ASN  |
| 29  | d     | 85  | ARG  |
| 29  | d     | 90  | ARG  |
| 29  | d     | 94  | GLU  |
| 29  | d     | 102 | LEU  |
| 29  | d     | 107 | THR  |
| 29  | d     | 116 | ASN  |
| 30  | e     | 11  | LYS  |
| 30  | e     | 21  | ILE  |
| 30  | e     | 22  | ARG  |
| 30  | e     | 24  | GLN  |
| 30  | e     | 30  | LYS  |
| 30  | e     | 32  | LYS  |
| 30  | e     | 46  | ARG  |
| 30  | e     | 48  | ARG  |
| 30  | e     | 64  | LYS  |
| 30  | e     | 78  | LEU  |
| 30  | e     | 91  | CYS  |
| 30  | e     | 104 | SER  |
| 30  | e     | 106 | LYS  |
| 30  | e     | 107 | ASN  |
| 30  | e     | 113 | GLU  |
| 31  | f     | 16  | ARG  |
| 31  | f     | 33  | VAL  |
| 31  | f     | 36  | ARG  |
| 31  | f     | 38  | GLU  |
| 31  | f     | 40  | GLU  |
| 31  | f     | 46  | ARG  |
| 31  | f     | 52  | LYS  |
| 31  | f     | 56  | ASN  |
| 31  | f     | 69  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | f     | 84  | VAL  |
| 31  | f     | 100 | ARG  |
| 31  | f     | 101 | ILE  |
| 32  | g     | 5   | LEU  |
| 32  | g     | 6   | THR  |
| 32  | g     | 11  | LEU  |
| 32  | g     | 14  | ASN  |
| 32  | g     | 15  | THR  |
| 32  | g     | 21  | ARG  |
| 32  | g     | 32  | TYR  |
| 32  | g     | 54  | ARG  |
| 32  | g     | 60  | ARG  |
| 32  | g     | 64  | LEU  |
| 32  | g     | 66  | ARG  |
| 32  | g     | 73  | HIS  |
| 32  | g     | 90  | ARG  |
| 32  | g     | 100 | GLN  |
| 32  | g     | 115 | LYS  |
| 33  | h     | 10  | ARG  |
| 33  | h     | 28  | LEU  |
| 33  | h     | 46  | LYS  |
| 33  | h     | 65  | GLN  |
| 33  | h     | 67  | GLU  |
| 33  | h     | 88  | THR  |
| 33  | h     | 89  | ARG  |
| 33  | h     | 97  | LYS  |
| 33  | h     | 104 | THR  |
| 33  | h     | 117 | ARG  |
| 33  | h     | 121 | VAL  |
| 33  | h     | 122 | LYS  |
| 34  | i     | 33  | LEU  |
| 34  | i     | 86  | LYS  |
| 34  | i     | 87  | ARG  |
| 34  | i     | 89  | GLU  |
| 34  | i     | 103 | LYS  |
| 35  | j     | 2   | THR  |
| 35  | j     | 3   | LYS  |
| 35  | j     | 15  | THR  |
| 35  | j     | 20  | ARG  |
| 35  | j     | 25  | LYS  |
| 35  | j     | 29  | LEU  |
| 35  | j     | 33  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | j     | 61  | THR  |
| 35  | j     | 63  | ARG  |
| 35  | j     | 68  | LYS  |
| 35  | j     | 79  | ARG  |
| 36  | k     | 18  | LYS  |
| 36  | k     | 29  | LYS  |
| 36  | k     | 31  | ASN  |
| 36  | k     | 37  | ARG  |
| 36  | k     | 39  | SER  |
| 36  | k     | 57  | LYS  |
| 36  | k     | 69  | LEU  |
| 36  | k     | 70  | LYS  |
| 37  | l     | 8   | ARG  |
| 37  | l     | 16  | LYS  |
| 37  | l     | 17  | GLN  |
| 37  | l     | 21  | ARG  |
| 37  | l     | 36  | ARG  |
| 37  | l     | 46  | ARG  |
| 37  | l     | 49  | LEU  |
| 38  | m     | 79  | GLU  |
| 38  | m     | 82  | LEU  |
| 38  | m     | 85  | LEU  |
| 38  | m     | 88  | LYS  |
| 38  | m     | 97  | ARG  |
| 38  | m     | 98  | LYS  |
| 38  | m     | 106 | ARG  |
| 38  | m     | 111 | ARG  |
| 38  | m     | 119 | ASN  |
| 39  | n     | 2   | ARG  |
| 39  | n     | 9   | ARG  |
| 39  | n     | 13  | LEU  |
| 39  | n     | 21  | ARG  |
| 40  | o     | 17  | LYS  |
| 40  | o     | 24  | THR  |
| 40  | o     | 26  | TYR  |
| 40  | o     | 31  | ASP  |
| 40  | o     | 33  | LEU  |
| 40  | o     | 36  | GLN  |
| 40  | o     | 55  | ILE  |
| 40  | o     | 61  | LYS  |
| 40  | o     | 69  | ARG  |
| 40  | o     | 82  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | o     | 89  | LYS  |
| 40  | o     | 96  | ASP  |
| 40  | o     | 102 | GLN  |
| 41  | p     | 16  | THR  |
| 41  | p     | 24  | LYS  |
| 41  | p     | 49  | ARG  |
| 41  | p     | 54  | ILE  |
| 41  | p     | 60  | CYS  |
| 41  | p     | 84  | ARG  |
| 42  | r     | 17  | LEU  |
| 42  | r     | 18  | ILE  |
| 42  | r     | 20  | ARG  |
| 42  | r     | 21  | ASN  |
| 42  | r     | 24  | THR  |
| 42  | r     | 26  | SER  |
| 42  | r     | 28  | GLU  |
| 42  | r     | 31  | ASN  |
| 42  | r     | 32  | LEU  |
| 42  | r     | 37  | SER  |
| 42  | r     | 39  | ARG  |
| 42  | r     | 41  | ASN  |
| 42  | r     | 60  | VAL  |
| 42  | r     | 67  | ARG  |
| 42  | r     | 70  | GLN  |
| 42  | r     | 71  | ARG  |
| 42  | r     | 80  | THR  |
| 42  | r     | 103 | HIS  |
| 42  | r     | 107 | ARG  |
| 42  | r     | 108 | MET  |
| 42  | r     | 118 | LEU  |
| 43  | s     | 38  | LYS  |
| 43  | s     | 44  | ARG  |
| 43  | s     | 62  | ARG  |
| 43  | s     | 68  | HIS  |
| 43  | s     | 94  | ASP  |
| 43  | s     | 133 | GLU  |
| 43  | s     | 146 | LYS  |
| 43  | s     | 149 | ARG  |
| 43  | s     | 174 | LEU  |
| 43  | s     | 185 | PHE  |
| 43  | s     | 191 | GLN  |
| 44  | t     | 1   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | t     | 14  | TYR  |
| 44  | t     | 40  | LYS  |
| 44  | t     | 95  | GLN  |
| 44  | t     | 104 | ILE  |
| 44  | t     | 106 | PHE  |
| 44  | t     | 114 | ARG  |
| 44  | t     | 123 | ARG  |
| 45  | 1     | 63  | SER  |
| 52  | AA    | 8   | LEU  |
| 52  | AA    | 9   | GLN  |
| 52  | AA    | 14  | ASP  |
| 52  | AA    | 23  | THR  |
| 52  | AA    | 32  | PHE  |
| 52  | AA    | 39  | TYR  |
| 52  | AA    | 41  | ARG  |
| 52  | AA    | 44  | ASP  |
| 52  | AA    | 46  | ILE  |
| 52  | AA    | 53  | ARG  |
| 52  | AA    | 58  | LEU  |
| 52  | AA    | 60  | LEU  |
| 52  | AA    | 79  | SER  |
| 52  | AA    | 111 | GLN  |
| 52  | AA    | 113 | GLN  |
| 52  | AA    | 131 | HIS  |
| 52  | AA    | 136 | GLU  |
| 52  | AA    | 142 | LEU  |
| 52  | AA    | 150 | THR  |
| 52  | AA    | 158 | ASP  |
| 52  | AA    | 178 | LEU  |
| 52  | AA    | 200 | ASP  |
| 53  | BB    | 27  | LYS  |
| 53  | BB    | 38  | MET  |
| 53  | BB    | 43  | ASN  |
| 53  | BB    | 47  | THR  |
| 53  | BB    | 51  | ARG  |
| 53  | BB    | 55  | THR  |
| 53  | BB    | 56  | LYS  |
| 53  | BB    | 63  | LYS  |
| 53  | BB    | 78  | GLU  |
| 53  | BB    | 82  | ARG  |
| 53  | BB    | 86  | LEU  |
| 53  | BB    | 105 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | BB    | 126 | ASP  |
| 53  | BB    | 134 | LEU  |
| 53  | BB    | 136 | ARG  |
| 53  | BB    | 139 | CYS  |
| 53  | BB    | 142 | PHE  |
| 53  | BB    | 143 | THR  |
| 53  | BB    | 150 | ILE  |
| 53  | BB    | 151 | ARG  |
| 53  | BB    | 157 | GLN  |
| 53  | BB    | 163 | GLN  |
| 53  | BB    | 169 | MET  |
| 53  | BB    | 212 | VAL  |
| 53  | BB    | 213 | ARG  |
| 54  | CC    | 66  | LEU  |
| 54  | CC    | 78  | LEU  |
| 54  | CC    | 79  | GLU  |
| 54  | CC    | 107 | LEU  |
| 54  | CC    | 110 | MET  |
| 54  | CC    | 114 | LYS  |
| 54  | CC    | 120 | GLN  |
| 54  | CC    | 121 | ARG  |
| 54  | CC    | 137 | VAL  |
| 54  | CC    | 152 | ARG  |
| 54  | CC    | 166 | ARG  |
| 54  | CC    | 167 | ARG  |
| 54  | CC    | 182 | CYS  |
| 54  | CC    | 183 | LYS  |
| 54  | CC    | 192 | LEU  |
| 54  | CC    | 202 | THR  |
| 54  | CC    | 208 | PRO  |
| 54  | CC    | 227 | TRP  |
| 54  | CC    | 230 | THR  |
| 54  | CC    | 233 | LEU  |
| 54  | CC    | 240 | THR  |
| 54  | CC    | 247 | THR  |
| 54  | CC    | 248 | TYR  |
| 54  | CC    | 251 | LEU  |
| 54  | CC    | 254 | ASP  |
| 54  | CC    | 257 | LYS  |
| 54  | CC    | 262 | THR  |
| 54  | CC    | 275 | LYS  |
| 55  | DD    | 9   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | DD    | 22  | ASN  |
| 55  | DD    | 31  | GLU  |
| 55  | DD    | 40  | ARG  |
| 55  | DD    | 42  | THR  |
| 55  | DD    | 59  | LEU  |
| 55  | DD    | 64  | ARG  |
| 55  | DD    | 72  | VAL  |
| 55  | DD    | 76  | ARG  |
| 55  | DD    | 94  | ARG  |
| 55  | DD    | 107 | TYR  |
| 55  | DD    | 113 | LEU  |
| 55  | DD    | 117 | ARG  |
| 55  | DD    | 120 | TYR  |
| 55  | DD    | 142 | LEU  |
| 55  | DD    | 154 | ASP  |
| 55  | DD    | 156 | LEU  |
| 55  | DD    | 167 | TYR  |
| 55  | DD    | 176 | LEU  |
| 55  | DD    | 190 | LEU  |
| 55  | DD    | 212 | GLU  |
| 55  | DD    | 221 | THR  |
| 56  | EE    | 3   | ARG  |
| 56  | EE    | 12  | VAL  |
| 56  | EE    | 17  | HIS  |
| 56  | EE    | 24  | THR  |
| 56  | EE    | 32  | SER  |
| 56  | EE    | 33  | THR  |
| 56  | EE    | 38  | LEU  |
| 56  | EE    | 42  | LEU  |
| 56  | EE    | 49  | ARG  |
| 56  | EE    | 53  | LYS  |
| 56  | EE    | 54  | TYR  |
| 56  | EE    | 59  | ASP  |
| 56  | EE    | 65  | CYS  |
| 56  | EE    | 66  | MET  |
| 56  | EE    | 67  | GLN  |
| 56  | EE    | 73  | ASP  |
| 56  | EE    | 92  | ILE  |
| 56  | EE    | 95  | THR  |
| 56  | EE    | 100 | ARG  |
| 56  | EE    | 105 | THR  |
| 56  | EE    | 123 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | EE    | 130 | PHE  |
| 56  | EE    | 148 | ARG  |
| 56  | EE    | 165 | GLU  |
| 56  | EE    | 169 | ILE  |
| 56  | EE    | 171 | ASP  |
| 56  | EE    | 174 | LYS  |
| 56  | EE    | 176 | ASP  |
| 56  | EE    | 181 | CYS  |
| 56  | EE    | 182 | MET  |
| 56  | EE    | 198 | ARG  |
| 56  | EE    | 205 | PHE  |
| 56  | EE    | 207 | VAL  |
| 56  | EE    | 220 | THR  |
| 56  | EE    | 222 | LEU  |
| 56  | EE    | 225 | ILE  |
| 56  | EE    | 240 | ARG  |
| 56  | EE    | 244 | ILE  |
| 56  | EE    | 250 | GLU  |
| 56  | EE    | 259 | LYS  |
| 57  | FF    | 35  | LEU  |
| 57  | FF    | 36  | GLN  |
| 57  | FF    | 43  | GLU  |
| 57  | FF    | 47  | LYS  |
| 57  | FF    | 63  | LYS  |
| 57  | FF    | 73  | THR  |
| 57  | FF    | 76  | MET  |
| 57  | FF    | 78  | MET  |
| 57  | FF    | 79  | HIS  |
| 57  | FF    | 88  | MET  |
| 57  | FF    | 89  | THR  |
| 57  | FF    | 91  | ARG  |
| 57  | FF    | 93  | VAL  |
| 57  | FF    | 95  | HIS  |
| 57  | FF    | 103 | LEU  |
| 57  | FF    | 106 | GLU  |
| 57  | FF    | 118 | ASN  |
| 57  | FF    | 125 | SER  |
| 57  | FF    | 126 | THR  |
| 57  | FF    | 130 | ARG  |
| 57  | FF    | 136 | ARG  |
| 57  | FF    | 141 | VAL  |
| 57  | FF    | 145 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | FF    | 149 | GLN  |
| 57  | FF    | 152 | TRP  |
| 57  | FF    | 160 | GLU  |
| 57  | FF    | 168 | THR  |
| 57  | FF    | 171 | GLU  |
| 57  | FF    | 173 | LEU  |
| 57  | FF    | 179 | ASN  |
| 57  | FF    | 187 | SER  |
| 57  | FF    | 190 | ILE  |
| 57  | FF    | 194 | ASP  |
| 57  | FF    | 203 | ASN  |
| 57  | FF    | 204 | ARG  |
| 58  | GG    | 14  | LYS  |
| 58  | GG    | 15  | LEU  |
| 58  | GG    | 30  | LYS  |
| 58  | GG    | 50  | VAL  |
| 58  | GG    | 56  | ASN  |
| 58  | GG    | 58  | LYS  |
| 58  | GG    | 64  | LYS  |
| 58  | GG    | 68  | LEU  |
| 58  | GG    | 76  | LEU  |
| 58  | GG    | 120 | ASP  |
| 58  | GG    | 121 | ILE  |
| 58  | GG    | 128 | THR  |
| 58  | GG    | 132 | ARG  |
| 58  | GG    | 136 | LYS  |
| 58  | GG    | 137 | ARG  |
| 58  | GG    | 143 | LYS  |
| 58  | GG    | 164 | LYS  |
| 58  | GG    | 172 | LYS  |
| 58  | GG    | 178 | ARG  |
| 58  | GG    | 183 | ARG  |
| 58  | GG    | 190 | ARG  |
| 58  | GG    | 191 | ARG  |
| 58  | GG    | 196 | LYS  |
| 58  | GG    | 208 | GLU  |
| 58  | GG    | 216 | ARG  |
| 58  | GG    | 224 | ARG  |
| 58  | GG    | 227 | GLN  |
| 58  | GG    | 235 | SER  |
| 59  | HH    | 7   | LYS  |
| 59  | HH    | 34  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | HH    | 35  | ASP  |
| 59  | HH    | 36  | LEU  |
| 59  | HH    | 72  | PHE  |
| 59  | HH    | 74  | LYS  |
| 59  | HH    | 82  | GLU  |
| 59  | HH    | 87  | PHE  |
| 59  | HH    | 95  | ILE  |
| 59  | HH    | 106 | ARG  |
| 59  | HH    | 109 | ARG  |
| 59  | HH    | 119 | SER  |
| 59  | HH    | 120 | ARG  |
| 59  | HH    | 121 | THR  |
| 59  | HH    | 145 | ARG  |
| 59  | HH    | 148 | LEU  |
| 59  | HH    | 153 | LEU  |
| 59  | HH    | 172 | THR  |
| 60  | II    | 12  | ARG  |
| 60  | II    | 21  | TYR  |
| 60  | II    | 23  | LYS  |
| 60  | II    | 52  | ASN  |
| 60  | II    | 70  | GLU  |
| 60  | II    | 74  | ARG  |
| 60  | II    | 76  | THR  |
| 60  | II    | 82  | VAL  |
| 60  | II    | 86  | SER  |
| 60  | II    | 88  | ASN  |
| 60  | II    | 96  | LEU  |
| 60  | II    | 100 | CYS  |
| 60  | II    | 111 | GLN  |
| 60  | II    | 115 | SER  |
| 60  | II    | 123 | ARG  |
| 60  | II    | 130 | THR  |
| 60  | II    | 140 | LYS  |
| 60  | II    | 153 | LYS  |
| 60  | II    | 162 | LEU  |
| 60  | II    | 168 | GLN  |
| 60  | II    | 196 | GLU  |
| 60  | II    | 203 | LYS  |
| 60  | II    | 206 | LYS  |
| 61  | JJ    | 21  | GLU  |
| 61  | JJ    | 29  | LEU  |
| 61  | JJ    | 39  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | JJ    | 42  | GLU  |
| 61  | JJ    | 45  | ARG  |
| 61  | JJ    | 65  | GLU  |
| 61  | JJ    | 69  | ARG  |
| 61  | JJ    | 86  | VAL  |
| 61  | JJ    | 101 | LYS  |
| 61  | JJ    | 110 | LEU  |
| 61  | JJ    | 116 | LYS  |
| 61  | JJ    | 127 | ARG  |
| 61  | JJ    | 131 | ARG  |
| 61  | JJ    | 133 | ARG  |
| 61  | JJ    | 135 | ILE  |
| 61  | JJ    | 136 | ARG  |
| 61  | JJ    | 138 | ARG  |
| 61  | JJ    | 162 | ARG  |
| 61  | JJ    | 172 | ARG  |
| 61  | JJ    | 176 | LYS  |
| 62  | KK    | 1   | MET  |
| 62  | KK    | 2   | LEU  |
| 62  | KK    | 13  | GLU  |
| 62  | KK    | 16  | PHE  |
| 62  | KK    | 43  | LEU  |
| 62  | KK    | 50  | GLN  |
| 62  | KK    | 60  | GLU  |
| 62  | KK    | 65  | ARG  |
| 62  | KK    | 66  | HIS  |
| 62  | KK    | 70  | TYR  |
| 62  | KK    | 74  | GLU  |
| 62  | KK    | 80  | ARG  |
| 62  | KK    | 89  | ILE  |
| 63  | LL    | 8   | ARG  |
| 63  | LL    | 16  | ILE  |
| 63  | LL    | 18  | GLN  |
| 63  | LL    | 22  | ARG  |
| 63  | LL    | 31  | GLU  |
| 63  | LL    | 40  | ILE  |
| 63  | LL    | 56  | ILE  |
| 63  | LL    | 66  | VAL  |
| 63  | LL    | 67  | SER  |
| 63  | LL    | 69  | ARG  |
| 63  | LL    | 74  | SER  |
| 63  | LL    | 76  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | LL    | 78  | THR  |
| 63  | LL    | 85  | THR  |
| 63  | LL    | 90  | ARG  |
| 63  | LL    | 91  | ASP  |
| 63  | LL    | 97  | ARG  |
| 63  | LL    | 106 | HIS  |
| 63  | LL    | 109 | MET  |
| 63  | LL    | 111 | VAL  |
| 63  | LL    | 114 | SER  |
| 63  | LL    | 121 | GLN  |
| 63  | LL    | 126 | VAL  |
| 63  | LL    | 134 | LEU  |
| 63  | LL    | 135 | SER  |
| 63  | LL    | 147 | LYS  |
| 64  | MM    | 12  | MET  |
| 64  | MM    | 26  | LEU  |
| 64  | MM    | 27  | ILE  |
| 64  | MM    | 31  | LEU  |
| 64  | MM    | 33  | ARG  |
| 64  | MM    | 36  | ARG  |
| 64  | MM    | 45  | ARG  |
| 64  | MM    | 48  | HIS  |
| 64  | MM    | 60  | MET  |
| 64  | MM    | 73  | GLN  |
| 64  | MM    | 74  | ILE  |
| 64  | MM    | 77  | ILE  |
| 64  | MM    | 78  | LYS  |
| 64  | MM    | 83  | LYS  |
| 64  | MM    | 88  | TRP  |
| 64  | MM    | 96  | ARG  |
| 64  | MM    | 101 | ARG  |
| 64  | MM    | 114 | TYR  |
| 64  | MM    | 127 | TYR  |
| 65  | NN    | 5   | HIS  |
| 65  | NN    | 13  | GLN  |
| 65  | NN    | 25  | TRP  |
| 65  | NN    | 27  | LYS  |
| 65  | NN    | 52  | VAL  |
| 65  | NN    | 57  | SER  |
| 65  | NN    | 64  | ARG  |
| 65  | NN    | 70  | LYS  |
| 65  | NN    | 75  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | NN    | 76  | LYS  |
| 65  | NN    | 78  | LYS  |
| 65  | NN    | 84  | LEU  |
| 65  | NN    | 86  | GLU  |
| 65  | NN    | 94  | LYS  |
| 65  | NN    | 102 | LEU  |
| 65  | NN    | 107 | LYS  |
| 65  | NN    | 110 | ASP  |
| 65  | NN    | 114 | ARG  |
| 65  | NN    | 120 | SER  |
| 65  | NN    | 121 | ARG  |
| 65  | NN    | 125 | LEU  |
| 65  | NN    | 142 | GLU  |
| 66  | OO    | 34  | PHE  |
| 66  | OO    | 38  | ASN  |
| 66  | OO    | 39  | ASP  |
| 66  | OO    | 50  | LYS  |
| 66  | OO    | 51  | GLU  |
| 66  | OO    | 53  | ILE  |
| 66  | OO    | 61  | LYS  |
| 66  | OO    | 65  | ASP  |
| 66  | OO    | 69  | SER  |
| 66  | OO    | 80  | ASP  |
| 66  | OO    | 81  | VAL  |
| 66  | OO    | 85  | CYS  |
| 66  | OO    | 100 | THR  |
| 66  | OO    | 104 | ARG  |
| 66  | OO    | 106 | LYS  |
| 66  | OO    | 107 | THR  |
| 66  | OO    | 121 | ARG  |
| 66  | OO    | 128 | ARG  |
| 66  | OO    | 130 | GLU  |
| 66  | OO    | 131 | ASP  |
| 66  | OO    | 133 | THR  |
| 66  | OO    | 137 | SER  |
| 66  | OO    | 142 | ARG  |
| 66  | OO    | 146 | ARG  |
| 66  | OO    | 151 | LEU  |
| 67  | PP    | 5   | GLU  |
| 67  | PP    | 7   | LYS  |
| 67  | PP    | 10  | ARG  |
| 67  | PP    | 17  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67  | PP    | 21  | ASP  |
| 67  | PP    | 28  | MET  |
| 67  | PP    | 29  | SER  |
| 67  | PP    | 30  | TYR  |
| 67  | PP    | 37  | TYR  |
| 67  | PP    | 40  | ARG  |
| 67  | PP    | 43  | ARG  |
| 67  | PP    | 44  | ARG  |
| 67  | PP    | 52  | LYS  |
| 67  | PP    | 65  | LYS  |
| 67  | PP    | 88  | GLU  |
| 67  | PP    | 100 | LYS  |
| 67  | PP    | 107 | ILE  |
| 67  | PP    | 121 | ILE  |
| 68  | QQ    | 20  | THR  |
| 68  | QQ    | 26  | LYS  |
| 68  | QQ    | 41  | MET  |
| 68  | QQ    | 47  | LEU  |
| 68  | QQ    | 73  | LYS  |
| 68  | QQ    | 85  | ARG  |
| 68  | QQ    | 89  | SER  |
| 68  | QQ    | 90  | LYS  |
| 68  | QQ    | 97  | GLN  |
| 68  | QQ    | 119 | LEU  |
| 68  | QQ    | 126 | ARG  |
| 68  | QQ    | 131 | LYS  |
| 68  | QQ    | 140 | ARG  |
| 68  | QQ    | 145 | TYR  |
| 68  | QQ    | 146 | ARG  |
| 69  | RR    | 43  | SER  |
| 69  | RR    | 47  | ARG  |
| 69  | RR    | 58  | MET  |
| 69  | RR    | 77  | GLU  |
| 69  | RR    | 78  | ARG  |
| 69  | RR    | 79  | GLU  |
| 69  | RR    | 82  | ASP  |
| 69  | RR    | 87  | GLU  |
| 69  | RR    | 88  | VAL  |
| 69  | RR    | 99  | ASP  |
| 69  | RR    | 101 | ASP  |
| 69  | RR    | 109 | LEU  |
| 69  | RR    | 118 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 69  | RR    | 121 | GLN  |
| 69  | RR    | 127 | ASN  |
| 70  | SS    | 7   | GLU  |
| 70  | SS    | 8   | LYS  |
| 70  | SS    | 10  | GLN  |
| 70  | SS    | 14  | ARG  |
| 70  | SS    | 17  | ASN  |
| 70  | SS    | 34  | LYS  |
| 70  | SS    | 52  | LEU  |
| 70  | SS    | 59  | LEU  |
| 70  | SS    | 63  | GLU  |
| 70  | SS    | 78  | LYS  |
| 70  | SS    | 81  | ASP  |
| 70  | SS    | 82  | TRP  |
| 70  | SS    | 86  | ARG  |
| 70  | SS    | 113 | ARG  |
| 70  | SS    | 115 | LYS  |
| 70  | SS    | 118 | ARG  |
| 70  | SS    | 131 | VAL  |
| 70  | SS    | 134 | GLN  |
| 70  | SS    | 136 | THR  |
| 71  | TT    | 4   | VAL  |
| 71  | TT    | 8   | ASP  |
| 71  | TT    | 28  | LEU  |
| 71  | TT    | 35  | ASP  |
| 71  | TT    | 37  | VAL  |
| 71  | TT    | 39  | LEU  |
| 71  | TT    | 62  | ARG  |
| 71  | TT    | 67  | ARG  |
| 71  | TT    | 74  | SER  |
| 71  | TT    | 84  | ARG  |
| 71  | TT    | 92  | PHE  |
| 71  | TT    | 93  | SER  |
| 71  | TT    | 102 | ARG  |
| 71  | TT    | 108 | GLU  |
| 71  | TT    | 121 | ARG  |
| 71  | TT    | 123 | LEU  |
| 71  | TT    | 124 | THR  |
| 71  | TT    | 128 | GLN  |
| 72  | UU    | 31  | SER  |
| 72  | UU    | 33  | GLU  |
| 72  | UU    | 36  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72  | UU    | 48  | LEU  |
| 72  | UU    | 49  | LYS  |
| 72  | UU    | 51  | LYS  |
| 72  | UU    | 55  | ARG  |
| 72  | UU    | 56  | MET  |
| 72  | UU    | 62  | ARG  |
| 72  | UU    | 68  | THR  |
| 72  | UU    | 81  | GLN  |
| 72  | UU    | 84  | ILE  |
| 72  | UU    | 93  | SER  |
| 72  | UU    | 111 | GLU  |
| 72  | UU    | 118 | ASP  |
| 73  | VV    | 9   | VAL  |
| 73  | VV    | 11  | LEU  |
| 73  | VV    | 31  | SER  |
| 73  | VV    | 38  | GLU  |
| 73  | VV    | 40  | ASP  |
| 73  | VV    | 74  | LYS  |
| 74  | WW    | 3   | ARG  |
| 74  | WW    | 22  | LYS  |
| 74  | WW    | 23  | ARG  |
| 74  | WW    | 25  | VAL  |
| 74  | WW    | 36  | ARG  |
| 74  | WW    | 74  | VAL  |
| 74  | WW    | 80  | ASP  |
| 74  | WW    | 83  | LEU  |
| 74  | WW    | 103 | VAL  |
| 74  | WW    | 104 | LEU  |
| 74  | WW    | 110 | ILE  |
| 74  | WW    | 111 | MET  |
| 74  | WW    | 117 | ARG  |
| 75  | XX    | 3   | LYS  |
| 75  | XX    | 4   | CYS  |
| 75  | XX    | 5   | ARG  |
| 75  | XX    | 9   | THR  |
| 75  | XX    | 12  | LYS  |
| 75  | XX    | 14  | ARG  |
| 75  | XX    | 29  | LYS  |
| 75  | XX    | 37  | LYS  |
| 75  | XX    | 61  | GLN  |
| 75  | XX    | 67  | ARG  |
| 75  | XX    | 68  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | XX    | 71  | ARG  |
| 75  | XX    | 98  | ASP  |
| 75  | XX    | 105 | PHE  |
| 75  | XX    | 112 | VAL  |
| 75  | XX    | 115 | ILE  |
| 75  | XX    | 123 | VAL  |
| 75  | XX    | 128 | VAL  |
| 75  | XX    | 130 | LEU  |
| 76  | YY    | 7   | ILE  |
| 76  | YY    | 10  | ARG  |
| 76  | YY    | 14  | THR  |
| 76  | YY    | 16  | ARG  |
| 76  | YY    | 20  | ARG  |
| 76  | YY    | 32  | LYS  |
| 76  | YY    | 40  | ILE  |
| 76  | YY    | 44  | LEU  |
| 76  | YY    | 46  | LYS  |
| 76  | YY    | 61  | ARG  |
| 76  | YY    | 62  | THR  |
| 76  | YY    | 69  | THR  |
| 76  | YY    | 72  | PHE  |
| 76  | YY    | 74  | MET  |
| 76  | YY    | 87  | PRO  |
| 76  | YY    | 98  | GLU  |
| 76  | YY    | 99  | LYS  |
| 76  | YY    | 100 | LYS  |
| 76  | YY    | 107 | ARG  |
| 76  | YY    | 111 | LYS  |
| 77  | ZZ    | 44  | LEU  |
| 77  | ZZ    | 74  | SER  |
| 77  | ZZ    | 83  | LEU  |
| 77  | ZZ    | 89  | GLN  |
| 77  | ZZ    | 93  | SER  |
| 77  | ZZ    | 110 | THR  |
| 77  | ZZ    | 114 | LYS  |
| 78  | aa    | 19  | GLN  |
| 78  | aa    | 23  | CYS  |
| 78  | aa    | 26  | CYS  |
| 78  | aa    | 33  | ASP  |
| 78  | aa    | 41  | ILE  |
| 78  | aa    | 51  | ARG  |
| 78  | aa    | 52  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | aa    | 94  | ASP  |
| 79  | bb    | 3   | LEU  |
| 79  | bb    | 17  | ARG  |
| 79  | bb    | 27  | SER  |
| 79  | bb    | 36  | LYS  |
| 79  | bb    | 37  | CYS  |
| 79  | bb    | 44  | THR  |
| 79  | bb    | 51  | GLN  |
| 79  | bb    | 60  | SER  |
| 79  | bb    | 63  | LEU  |
| 79  | bb    | 72  | ARG  |
| 79  | bb    | 81  | ARG  |
| 79  | bb    | 83  | GLN  |
| 79  | bb    | 84  | HIS  |
| 80  | cc    | 31  | ARG  |
| 80  | cc    | 34  | PHE  |
| 80  | cc    | 35  | MET  |
| 80  | cc    | 58  | LEU  |
| 80  | cc    | 60  | GLU  |
| 80  | cc    | 61  | SER  |
| 80  | cc    | 62  | GLU  |
| 80  | cc    | 63  | ARG  |
| 80  | cc    | 67  | ARG  |
| 80  | cc    | 68  | LEU  |
| 81  | dd    | 5   | GLN  |
| 81  | dd    | 6   | LEU  |
| 81  | dd    | 16  | GLN  |
| 81  | dd    | 26  | ASN  |
| 81  | dd    | 27  | ARG  |
| 81  | dd    | 39  | CYS  |
| 81  | dd    | 54  | LYS  |
| 82  | ee    | 15  | GLN  |
| 82  | ee    | 18  | LYS  |
| 82  | ee    | 24  | LYS  |
| 82  | ee    | 34  | ARG  |
| 82  | ee    | 36  | MET  |
| 82  | ee    | 41  | ARG  |
| 82  | ee    | 43  | VAL  |
| 82  | ee    | 52  | LYS  |
| 83  | ff    | 81  | THR  |
| 84  | gg    | 20  | GLN  |
| 84  | gg    | 29  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 84  | gg    | 36  | ARG  |
| 84  | gg    | 44  | LYS  |
| 84  | gg    | 47  | ARG  |
| 84  | gg    | 49  | GLU  |
| 84  | gg    | 63  | SER  |
| 84  | gg    | 64  | HIS  |
| 84  | gg    | 65  | PHE  |
| 84  | gg    | 93  | THR  |
| 84  | gg    | 99  | ARG  |
| 84  | gg    | 100 | ARG  |
| 84  | gg    | 107 | ASP  |
| 84  | gg    | 143 | GLN  |
| 84  | gg    | 156 | PHE  |
| 84  | gg    | 172 | LYS  |
| 84  | gg    | 186 | THR  |
| 84  | gg    | 234 | ASP  |
| 84  | gg    | 282 | GLU  |
| 84  | gg    | 289 | LEU  |
| 84  | gg    | 298 | LEU  |
| 84  | gg    | 306 | LEU  |
| 86  | ii    | 45  | ILE  |
| 86  | ii    | 61  | ASN  |
| 86  | ii    | 65  | ARG  |
| 86  | ii    | 67  | ASN  |
| 86  | ii    | 80  | GLN  |
| 86  | ii    | 82  | LEU  |
| 86  | ii    | 86  | ASN  |
| 86  | ii    | 103 | GLU  |
| 86  | ii    | 111 | ASN  |
| 86  | ii    | 112 | ILE  |
| 86  | ii    | 128 | ASP  |
| 86  | ii    | 136 | LEU  |
| 86  | ii    | 139 | LEU  |
| 86  | ii    | 164 | ASN  |
| 86  | ii    | 165 | THR  |
| 86  | ii    | 167 | GLU  |
| 86  | ii    | 179 | LYS  |
| 86  | ii    | 180 | HIS  |
| 86  | ii    | 182 | ARG  |
| 86  | ii    | 186 | SER  |
| 86  | ii    | 211 | GLN  |
| 86  | ii    | 212 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 86  | ii    | 231 | ASP  |
| 86  | ii    | 232 | PHE  |
| 86  | ii    | 241 | MET  |
| 86  | ii    | 246 | LEU  |
| 86  | ii    | 255 | ASP  |
| 86  | ii    | 300 | LYS  |
| 86  | ii    | 333 | LEU  |
| 86  | ii    | 339 | GLU  |
| 86  | ii    | 340 | GLU  |
| 86  | ii    | 361 | GLU  |
| 86  | ii    | 368 | LEU  |
| 86  | ii    | 415 | TYR  |
| 87  | jj    | 52  | GLU  |
| 87  | jj    | 75  | LEU  |
| 87  | jj    | 90  | ASN  |
| 87  | jj    | 106 | LEU  |
| 87  | jj    | 131 | LEU  |
| 87  | jj    | 161 | GLU  |
| 87  | jj    | 248 | ASP  |
| 87  | jj    | 250 | LYS  |
| 87  | jj    | 289 | LEU  |
| 87  | jj    | 296 | TYR  |
| 87  | jj    | 320 | GLU  |
| 87  | jj    | 374 | ILE  |
| 87  | jj    | 399 | ASP  |
| 87  | jj    | 411 | TYR  |
| 87  | jj    | 455 | ILE  |
| 87  | jj    | 486 | ASP  |
| 87  | jj    | 494 | SER  |
| 87  | jj    | 567 | ARG  |
| 87  | jj    | 574 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 217 | GLN  |
| 7   | G     | 29  | ASN  |
| 42  | r     | 103 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 46  | 2     | 74/76 (97%)     | 20 (27%)          | 1 (1%)          |
| 47  | 3     | 72/75 (96%)     | 36 (50%)          | 7 (9%)          |
| 48  | 5     | 3645/3662 (99%) | 1179 (32%)        | 269 (7%)        |
| 49  | 7     | 119/120 (99%)   | 19 (15%)          | 1 (0%)          |
| 50  | 8     | 155/156 (99%)   | 52 (33%)          | 6 (3%)          |
| 51  | 9     | 1711/1719 (99%) | 608 (35%)         | 129 (7%)        |
| 85  | hh    | 11/12 (91%)     | 7 (63%)           | 0               |
| All | All   | 5787/5820 (99%) | 1921 (33%)        | 413 (7%)        |

All (1921) RNA backbone outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 46  | 2     | 7     | G    |
| 46  | 2     | 8     | U    |
| 46  | 2     | 9     | A    |
| 46  | 2     | 13    | U    |
| 46  | 2     | 16    | C    |
| 46  | 2     | 19    | G    |
| 46  | 2     | 20(A) | U    |
| 46  | 2     | 21    | A    |
| 46  | 2     | 31    | C    |
| 46  | 2     | 35    | A    |
| 46  | 2     | 42    | A    |
| 46  | 2     | 47    | U    |
| 46  | 2     | 49    | C    |
| 46  | 2     | 58    | A    |
| 46  | 2     | 60    | A    |
| 46  | 2     | 61    | C    |
| 46  | 2     | 67    | G    |
| 46  | 2     | 72    | C    |
| 46  | 2     | 75    | C    |
| 46  | 2     | 76    | A    |
| 47  | 3     | 2     | C    |
| 47  | 3     | 5     | G    |
| 47  | 3     | 7     | A    |
| 47  | 3     | 8     | U    |
| 47  | 3     | 9     | A    |
| 47  | 3     | 10    | G    |
| 47  | 3     | 13    | C    |
| 47  | 3     | 21    | A    |
| 47  | 3     | 22    | G    |
| 47  | 3     | 29    | A    |
| 47  | 3     | 30    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 3     | 31  | A    |
| 47  | 3     | 34  | U    |
| 47  | 3     | 35  | U    |
| 47  | 3     | 38  | A    |
| 47  | 3     | 39  | U    |
| 47  | 3     | 41  | U    |
| 47  | 3     | 42  | G    |
| 47  | 3     | 47  | U    |
| 47  | 3     | 48  | C    |
| 47  | 3     | 49  | C    |
| 47  | 3     | 58  | A    |
| 47  | 3     | 60  | U    |
| 47  | 3     | 61  | C    |
| 47  | 3     | 63  | C    |
| 47  | 3     | 65  | G    |
| 47  | 3     | 67  | U    |
| 47  | 3     | 68  | C    |
| 47  | 3     | 69  | G    |
| 47  | 3     | 70  | G    |
| 47  | 3     | 71  | G    |
| 47  | 3     | 72  | C    |
| 47  | 3     | 73  | G    |
| 47  | 3     | 74  | C    |
| 47  | 3     | 75  | C    |
| 47  | 3     | 76  | A    |
| 48  | 5     | 2   | G    |
| 48  | 5     | 8   | U    |
| 48  | 5     | 9   | C    |
| 48  | 5     | 10  | A    |
| 48  | 5     | 12  | A    |
| 48  | 5     | 13  | U    |
| 48  | 5     | 21  | G    |
| 48  | 5     | 25  | A    |
| 48  | 5     | 30  | C    |
| 48  | 5     | 39  | A    |
| 48  | 5     | 42  | A    |
| 48  | 5     | 43  | U    |
| 48  | 5     | 44  | A    |
| 48  | 5     | 48  | G    |
| 48  | 5     | 49  | U    |
| 48  | 5     | 56  | A    |
| 48  | 5     | 58  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 5     | 59  | A    |
| 48  | 5     | 64  | A    |
| 48  | 5     | 65  | A    |
| 48  | 5     | 69  | A    |
| 48  | 5     | 71  | C    |
| 48  | 5     | 72  | C    |
| 48  | 5     | 73  | A    |
| 48  | 5     | 74  | G    |
| 48  | 5     | 91  | G    |
| 48  | 5     | 93  | G    |
| 48  | 5     | 94  | A    |
| 48  | 5     | 95  | G    |
| 48  | 5     | 108 | A    |
| 48  | 5     | 109 | G    |
| 48  | 5     | 110 | C    |
| 48  | 5     | 116 | G    |
| 48  | 5     | 118 | C    |
| 48  | 5     | 119 | G    |
| 48  | 5     | 120 | A    |
| 48  | 5     | 121 | A    |
| 48  | 5     | 126 | C    |
| 48  | 5     | 128 | C    |
| 48  | 5     | 129 | C    |
| 48  | 5     | 134 | G    |
| 48  | 5     | 135 | G    |
| 48  | 5     | 136 | C    |
| 48  | 5     | 143 | C    |
| 48  | 5     | 144 | G    |
| 48  | 5     | 146 | G    |
| 48  | 5     | 157 | U    |
| 48  | 5     | 159 | C    |
| 48  | 5     | 160 | G    |
| 48  | 5     | 161 | G    |
| 48  | 5     | 164 | G    |
| 48  | 5     | 166 | C    |
| 48  | 5     | 167 | C    |
| 48  | 5     | 170 | C    |
| 48  | 5     | 171 | U    |
| 48  | 5     | 172 | C    |
| 48  | 5     | 173 | C    |
| 48  | 5     | 174 | C    |
| 48  | 5     | 175 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 5     | 177 | G    |
| 48  | 5     | 183 | C    |
| 48  | 5     | 184 | U    |
| 48  | 5     | 185 | C    |
| 48  | 5     | 186 | G    |
| 48  | 5     | 187 | U    |
| 48  | 5     | 188 | G    |
| 48  | 5     | 189 | G    |
| 48  | 5     | 197 | A    |
| 48  | 5     | 200 | U    |
| 48  | 5     | 201 | C    |
| 48  | 5     | 203 | U    |
| 48  | 5     | 205 | C    |
| 48  | 5     | 209 | U    |
| 48  | 5     | 210 | C    |
| 48  | 5     | 216 | C    |
| 48  | 5     | 217 | C    |
| 48  | 5     | 218 | A    |
| 48  | 5     | 219 | G    |
| 48  | 5     | 220 | C    |
| 48  | 5     | 221 | C    |
| 48  | 5     | 224 | U    |
| 48  | 5     | 226 | G    |
| 48  | 5     | 227 | A    |
| 48  | 5     | 233 | U    |
| 48  | 5     | 234 | G    |
| 48  | 5     | 246 | G    |
| 48  | 5     | 253 | G    |
| 48  | 5     | 255 | C    |
| 48  | 5     | 257 | C    |
| 48  | 5     | 265 | C    |
| 48  | 5     | 266 | C    |
| 48  | 5     | 267 | G    |
| 48  | 5     | 272 | U    |
| 48  | 5     | 276 | C    |
| 48  | 5     | 277 | G    |
| 48  | 5     | 278 | G    |
| 48  | 5     | 280 | G    |
| 48  | 5     | 286 | U    |
| 48  | 5     | 296 | A    |
| 48  | 5     | 297 | U    |
| 48  | 5     | 300 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 5     | 306 | A    |
| 48  | 5     | 309 | C    |
| 48  | 5     | 315 | G    |
| 48  | 5     | 316 | U    |
| 48  | 5     | 319 | A    |
| 48  | 5     | 321 | U    |
| 48  | 5     | 322 | C    |
| 48  | 5     | 326 | C    |
| 48  | 5     | 328 | A    |
| 48  | 5     | 334 | A    |
| 48  | 5     | 337 | U    |
| 48  | 5     | 340 | C    |
| 48  | 5     | 347 | A    |
| 48  | 5     | 349 | A    |
| 48  | 5     | 350 | C    |
| 48  | 5     | 353 | A    |
| 48  | 5     | 357 | U    |
| 48  | 5     | 361 | C    |
| 48  | 5     | 362 | A    |
| 48  | 5     | 363 | A    |
| 48  | 5     | 385 | A    |
| 48  | 5     | 386 | A    |
| 48  | 5     | 387 | G    |
| 48  | 5     | 399 | G    |
| 48  | 5     | 405 | U    |
| 48  | 5     | 406 | C    |
| 48  | 5     | 407 | A    |
| 48  | 5     | 409 | G    |
| 48  | 5     | 410 | A    |
| 48  | 5     | 412 | G    |
| 48  | 5     | 413 | G    |
| 48  | 5     | 424 | U    |
| 48  | 5     | 429 | A    |
| 48  | 5     | 431 | G    |
| 48  | 5     | 432 | U    |
| 48  | 5     | 434 | A    |
| 48  | 5     | 446 | C    |
| 48  | 5     | 448 | G    |
| 48  | 5     | 449 | C    |
| 48  | 5     | 451 | C    |
| 48  | 5     | 452 | A    |
| 48  | 5     | 453 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 5     | 454 | U    |
| 48  | 5     | 455 | C    |
| 48  | 5     | 458 | C    |
| 48  | 5     | 465 | G    |
| 48  | 5     | 467 | U    |
| 48  | 5     | 468 | U    |
| 48  | 5     | 469 | C    |
| 48  | 5     | 470 | A    |
| 48  | 5     | 473 | C    |
| 48  | 5     | 485 | C    |
| 48  | 5     | 486 | C    |
| 48  | 5     | 487 | G    |
| 48  | 5     | 498 | C    |
| 48  | 5     | 499 | G    |
| 48  | 5     | 500 | G    |
| 48  | 5     | 501 | C    |
| 48  | 5     | 502 | C    |
| 48  | 5     | 503 | C    |
| 48  | 5     | 504 | G    |
| 48  | 5     | 506 | C    |
| 48  | 5     | 509 | A    |
| 48  | 5     | 510 | U    |
| 48  | 5     | 513 | U    |
| 48  | 5     | 514 | U    |
| 48  | 5     | 515 | C    |
| 48  | 5     | 519 | C    |
| 48  | 5     | 649 | A    |
| 48  | 5     | 654 | C    |
| 48  | 5     | 655 | C    |
| 48  | 5     | 663 | G    |
| 48  | 5     | 664 | G    |
| 48  | 5     | 665 | C    |
| 48  | 5     | 666 | G    |
| 48  | 5     | 667 | A    |
| 48  | 5     | 668 | C    |
| 48  | 5     | 682 | G    |
| 48  | 5     | 684 | G    |
| 48  | 5     | 685 | C    |
| 48  | 5     | 686 | A    |
| 48  | 5     | 690 | C    |
| 48  | 5     | 694 | C    |
| 48  | 5     | 695 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 5     | 696 | C    |
| 48  | 5     | 697 | G    |
| 48  | 5     | 701 | G    |
| 48  | 5     | 703 | G    |
| 48  | 5     | 707 | C    |
| 48  | 5     | 718 | C    |
| 48  | 5     | 721 | G    |
| 48  | 5     | 722 | G    |
| 48  | 5     | 724 | C    |
| 48  | 5     | 728 | U    |
| 48  | 5     | 729 | G    |
| 48  | 5     | 730 | G    |
| 48  | 5     | 737 | C    |
| 48  | 5     | 742 | G    |
| 48  | 5     | 745 | G    |
| 48  | 5     | 746 | A    |
| 48  | 5     | 747 | A    |
| 48  | 5     | 748 | G    |
| 48  | 5     | 749 | G    |
| 48  | 5     | 756 | G    |
| 48  | 5     | 911 | U    |
| 48  | 5     | 914 | U    |
| 48  | 5     | 915 | A    |
| 48  | 5     | 917 | A    |
| 48  | 5     | 918 | G    |
| 48  | 5     | 919 | C    |
| 48  | 5     | 920 | C    |
| 48  | 5     | 925 | C    |
| 48  | 5     | 927 | G    |
| 48  | 5     | 928 | C    |
| 48  | 5     | 929 | A    |
| 48  | 5     | 930 | G    |
| 48  | 5     | 931 | C    |
| 48  | 5     | 932 | A    |
| 48  | 5     | 933 | G    |
| 48  | 5     | 934 | C    |
| 48  | 5     | 935 | A    |
| 48  | 5     | 936 | C    |
| 48  | 5     | 937 | U    |
| 48  | 5     | 938 | C    |
| 48  | 5     | 939 | G    |
| 48  | 5     | 940 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 942  | G    |
| 48  | 5     | 943  | A    |
| 48  | 5     | 944  | A    |
| 48  | 5     | 945  | U    |
| 48  | 5     | 946  | C    |
| 48  | 5     | 947  | C    |
| 48  | 5     | 957  | G    |
| 48  | 5     | 958  | G    |
| 48  | 5     | 960  | A    |
| 48  | 5     | 961  | G    |
| 48  | 5     | 962  | C    |
| 48  | 5     | 963  | G    |
| 48  | 5     | 964  | A    |
| 48  | 5     | 965  | G    |
| 48  | 5     | 966  | A    |
| 48  | 5     | 967  | C    |
| 48  | 5     | 968  | C    |
| 48  | 5     | 969  | C    |
| 48  | 5     | 970  | G    |
| 48  | 5     | 971  | U    |
| 48  | 5     | 972  | C    |
| 48  | 5     | 973  | G    |
| 48  | 5     | 976  | G    |
| 48  | 5     | 977  | C    |
| 48  | 5     | 978  | G    |
| 48  | 5     | 979  | C    |
| 48  | 5     | 982  | U    |
| 48  | 5     | 983  | C    |
| 48  | 5     | 984  | C    |
| 48  | 5     | 989  | U    |
| 48  | 5     | 990  | C    |
| 48  | 5     | 992  | C    |
| 48  | 5     | 1051 | G    |
| 48  | 5     | 1070 | G    |
| 48  | 5     | 1072 | C    |
| 48  | 5     | 1073 | G    |
| 48  | 5     | 1075 | G    |
| 48  | 5     | 1076 | C    |
| 48  | 5     | 1083 | U    |
| 48  | 5     | 1097 | C    |
| 48  | 5     | 1175 | A    |
| 48  | 5     | 1176 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1177 | U    |
| 48  | 5     | 1181 | C    |
| 48  | 5     | 1182 | C    |
| 48  | 5     | 1183 | C    |
| 48  | 5     | 1193 | C    |
| 48  | 5     | 1204 | C    |
| 48  | 5     | 1209 | U    |
| 48  | 5     | 1211 | G    |
| 48  | 5     | 1212 | G    |
| 48  | 5     | 1214 | C    |
| 48  | 5     | 1215 | C    |
| 48  | 5     | 1219 | G    |
| 48  | 5     | 1221 | G    |
| 48  | 5     | 1222 | A    |
| 48  | 5     | 1233 | G    |
| 48  | 5     | 1234 | G    |
| 48  | 5     | 1235 | G    |
| 48  | 5     | 1236 | C    |
| 48  | 5     | 1237 | C    |
| 48  | 5     | 1238 | A    |
| 48  | 5     | 1239 | C    |
| 48  | 5     | 1240 | G    |
| 48  | 5     | 1241 | C    |
| 48  | 5     | 1242 | G    |
| 48  | 5     | 1243 | C    |
| 48  | 5     | 1244 | G    |
| 48  | 5     | 1245 | C    |
| 48  | 5     | 1255 | A    |
| 48  | 5     | 1256 | G    |
| 48  | 5     | 1259 | G    |
| 48  | 5     | 1266 | G    |
| 48  | 5     | 1267 | C    |
| 48  | 5     | 1268 | G    |
| 48  | 5     | 1269 | G    |
| 48  | 5     | 1270 | A    |
| 48  | 5     | 1272 | C    |
| 48  | 5     | 1273 | G    |
| 48  | 5     | 1274 | A    |
| 48  | 5     | 1275 | G    |
| 48  | 5     | 1279 | A    |
| 48  | 5     | 1280 | C    |
| 48  | 5     | 1281 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1285 | U    |
| 48  | 5     | 1286 | C    |
| 48  | 5     | 1287 | G    |
| 48  | 5     | 1288 | G    |
| 48  | 5     | 1289 | C    |
| 48  | 5     | 1293 | G    |
| 48  | 5     | 1294 | A    |
| 48  | 5     | 1295 | C    |
| 48  | 5     | 1296 | G    |
| 48  | 5     | 1297 | U    |
| 48  | 5     | 1301 | C    |
| 48  | 5     | 1303 | A    |
| 48  | 5     | 1304 | C    |
| 48  | 5     | 1313 | C    |
| 48  | 5     | 1326 | A    |
| 48  | 5     | 1330 | A    |
| 48  | 5     | 1337 | A    |
| 48  | 5     | 1344 | C    |
| 48  | 5     | 1354 | A    |
| 48  | 5     | 1358 | G    |
| 48  | 5     | 1364 | U    |
| 48  | 5     | 1365 | C    |
| 48  | 5     | 1366 | G    |
| 48  | 5     | 1367 | C    |
| 48  | 5     | 1368 | A    |
| 48  | 5     | 1369 | C    |
| 48  | 5     | 1370 | G    |
| 48  | 5     | 1371 | A    |
| 48  | 5     | 1372 | A    |
| 48  | 5     | 1376 | C    |
| 48  | 5     | 1377 | G    |
| 48  | 5     | 1378 | C    |
| 48  | 5     | 1379 | C    |
| 48  | 5     | 1380 | G    |
| 48  | 5     | 1381 | U    |
| 48  | 5     | 1387 | A    |
| 48  | 5     | 1390 | G    |
| 48  | 5     | 1394 | G    |
| 48  | 5     | 1397 | A    |
| 48  | 5     | 1398 | A    |
| 48  | 5     | 1399 | G    |
| 48  | 5     | 1407 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1408 | G    |
| 48  | 5     | 1409 | C    |
| 48  | 5     | 1410 | U    |
| 48  | 5     | 1411 | C    |
| 48  | 5     | 1413 | C    |
| 48  | 5     | 1414 | C    |
| 48  | 5     | 1416 | G    |
| 48  | 5     | 1418 | C    |
| 48  | 5     | 1420 | A    |
| 48  | 5     | 1421 | G    |
| 48  | 5     | 1429 | C    |
| 48  | 5     | 1432 | G    |
| 48  | 5     | 1435 | G    |
| 48  | 5     | 1436 | C    |
| 48  | 5     | 1439 | C    |
| 48  | 5     | 1440 | U    |
| 48  | 5     | 1441 | C    |
| 48  | 5     | 1442 | C    |
| 48  | 5     | 1445 | U    |
| 48  | 5     | 1446 | C    |
| 48  | 5     | 1448 | G    |
| 48  | 5     | 1449 | C    |
| 48  | 5     | 1455 | G    |
| 48  | 5     | 1456 | C    |
| 48  | 5     | 1457 | G    |
| 48  | 5     | 1475 | G    |
| 48  | 5     | 1477 | C    |
| 48  | 5     | 1478 | C    |
| 48  | 5     | 1481 | C    |
| 48  | 5     | 1482 | G    |
| 48  | 5     | 1483 | C    |
| 48  | 5     | 1484 | G    |
| 48  | 5     | 1485 | C    |
| 48  | 5     | 1486 | C    |
| 48  | 5     | 1489 | G    |
| 48  | 5     | 1497 | A    |
| 48  | 5     | 1498 | G    |
| 48  | 5     | 1501 | C    |
| 48  | 5     | 1502 | G    |
| 48  | 5     | 1504 | G    |
| 48  | 5     | 1514 | U    |
| 48  | 5     | 1516 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1518 | A    |
| 48  | 5     | 1523 | A    |
| 48  | 5     | 1524 | A    |
| 48  | 5     | 1533 | A    |
| 48  | 5     | 1534 | A    |
| 48  | 5     | 1547 | A    |
| 48  | 5     | 1563 | A    |
| 48  | 5     | 1564 | A    |
| 48  | 5     | 1566 | C    |
| 48  | 5     | 1568 | C    |
| 48  | 5     | 1578 | U    |
| 48  | 5     | 1582 | U    |
| 48  | 5     | 1586 | G    |
| 48  | 5     | 1591 | U    |
| 48  | 5     | 1592 | G    |
| 48  | 5     | 1596 | U    |
| 48  | 5     | 1602 | U    |
| 48  | 5     | 1612 | G    |
| 48  | 5     | 1613 | A    |
| 48  | 5     | 1614 | C    |
| 48  | 5     | 1624 | G    |
| 48  | 5     | 1625 | G    |
| 48  | 5     | 1631 | A    |
| 48  | 5     | 1633 | G    |
| 48  | 5     | 1634 | A    |
| 48  | 5     | 1636 | U    |
| 48  | 5     | 1638 | A    |
| 48  | 5     | 1641 | G    |
| 48  | 5     | 1654 | G    |
| 48  | 5     | 1655 | C    |
| 48  | 5     | 1656 | U    |
| 48  | 5     | 1661 | C    |
| 48  | 5     | 1670 | G    |
| 48  | 5     | 1676 | C    |
| 48  | 5     | 1677 | U    |
| 48  | 5     | 1691 | G    |
| 48  | 5     | 1692 | C    |
| 48  | 5     | 1696 | C    |
| 48  | 5     | 1697 | G    |
| 48  | 5     | 1698 | C    |
| 48  | 5     | 1699 | A    |
| 48  | 5     | 1719 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1720 | C    |
| 48  | 5     | 1721 | G    |
| 48  | 5     | 1722 | C    |
| 48  | 5     | 1724 | G    |
| 48  | 5     | 1725 | U    |
| 48  | 5     | 1733 | G    |
| 48  | 5     | 1734 | G    |
| 48  | 5     | 1735 | U    |
| 48  | 5     | 1742 | A    |
| 48  | 5     | 1746 | A    |
| 48  | 5     | 1750 | G    |
| 48  | 5     | 1753 | G    |
| 48  | 5     | 1754 | U    |
| 48  | 5     | 1755 | C    |
| 48  | 5     | 1756 | U    |
| 48  | 5     | 1757 | U    |
| 48  | 5     | 1758 | G    |
| 48  | 5     | 1760 | G    |
| 48  | 5     | 1761 | G    |
| 48  | 5     | 1764 | G    |
| 48  | 5     | 1767 | A    |
| 48  | 5     | 1768 | C    |
| 48  | 5     | 1772 | C    |
| 48  | 5     | 1776 | A    |
| 48  | 5     | 1777 | C    |
| 48  | 5     | 1781 | U    |
| 48  | 5     | 1787 | A    |
| 48  | 5     | 1799 | G    |
| 48  | 5     | 1800 | U    |
| 48  | 5     | 1803 | G    |
| 48  | 5     | 1804 | A    |
| 48  | 5     | 1805 | A    |
| 48  | 5     | 1812 | C    |
| 48  | 5     | 1815 | G    |
| 48  | 5     | 1818 | G    |
| 48  | 5     | 1819 | G    |
| 48  | 5     | 1820 | C    |
| 48  | 5     | 1821 | G    |
| 48  | 5     | 1822 | U    |
| 48  | 5     | 1828 | C    |
| 48  | 5     | 1830 | G    |
| 48  | 5     | 1832 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1833 | G    |
| 48  | 5     | 1834 | U    |
| 48  | 5     | 1835 | G    |
| 48  | 5     | 1836 | G    |
| 48  | 5     | 1847 | C    |
| 48  | 5     | 1848 | C    |
| 48  | 5     | 1855 | G    |
| 48  | 5     | 1867 | A    |
| 48  | 5     | 1869 | G    |
| 48  | 5     | 1882 | U    |
| 48  | 5     | 1885 | G    |
| 48  | 5     | 1886 | G    |
| 48  | 5     | 1889 | U    |
| 48  | 5     | 1892 | A    |
| 48  | 5     | 1897 | A    |
| 48  | 5     | 1899 | G    |
| 48  | 5     | 1900 | C    |
| 48  | 5     | 1910 | G    |
| 48  | 5     | 1918 | U    |
| 48  | 5     | 1919 | G    |
| 48  | 5     | 1920 | C    |
| 48  | 5     | 1921 | C    |
| 48  | 5     | 1922 | G    |
| 48  | 5     | 1923 | A    |
| 48  | 5     | 1931 | C    |
| 48  | 5     | 1947 | U    |
| 48  | 5     | 1952 | G    |
| 48  | 5     | 1955 | G    |
| 48  | 5     | 1956 | A    |
| 48  | 5     | 1957 | U    |
| 48  | 5     | 1958 | A    |
| 48  | 5     | 1959 | U    |
| 48  | 5     | 1960 | A    |
| 48  | 5     | 1961 | G    |
| 48  | 5     | 1964 | A    |
| 48  | 5     | 1968 | G    |
| 48  | 5     | 1969 | G    |
| 48  | 5     | 1975 | G    |
| 48  | 5     | 1976 | G    |
| 48  | 5     | 1977 | C    |
| 48  | 5     | 1979 | A    |
| 48  | 5     | 1980 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1981 | G    |
| 48  | 5     | 1983 | A    |
| 48  | 5     | 1984 | A    |
| 48  | 5     | 1985 | G    |
| 48  | 5     | 1986 | U    |
| 48  | 5     | 1987 | C    |
| 48  | 5     | 1988 | G    |
| 48  | 5     | 1990 | A    |
| 48  | 5     | 1991 | A    |
| 48  | 5     | 1992 | U    |
| 48  | 5     | 1993 | C    |
| 48  | 5     | 1997 | U    |
| 48  | 5     | 1998 | A    |
| 48  | 5     | 2001 | G    |
| 48  | 5     | 2002 | A    |
| 48  | 5     | 2003 | G    |
| 48  | 5     | 2004 | U    |
| 48  | 5     | 2005 | G    |
| 48  | 5     | 2008 | U    |
| 48  | 5     | 2010 | A    |
| 48  | 5     | 2011 | C    |
| 48  | 5     | 2019 | C    |
| 48  | 5     | 2020 | U    |
| 48  | 5     | 2021 | G    |
| 48  | 5     | 2024 | G    |
| 48  | 5     | 2025 | A    |
| 48  | 5     | 2026 | A    |
| 48  | 5     | 2027 | U    |
| 48  | 5     | 2028 | C    |
| 48  | 5     | 2044 | U    |
| 48  | 5     | 2046 | G    |
| 48  | 5     | 2047 | A    |
| 48  | 5     | 2048 | U    |
| 48  | 5     | 2052 | G    |
| 48  | 5     | 2055 | G    |
| 48  | 5     | 2056 | G    |
| 48  | 5     | 2062 | C    |
| 48  | 5     | 2064 | G    |
| 48  | 5     | 2068 | C    |
| 48  | 5     | 2069 | A    |
| 48  | 5     | 2070 | U    |
| 48  | 5     | 2071 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2079 | G    |
| 48  | 5     | 2084 | C    |
| 48  | 5     | 2085 | G    |
| 48  | 5     | 2089 | G    |
| 48  | 5     | 2090 | U    |
| 48  | 5     | 2091 | C    |
| 48  | 5     | 2092 | G    |
| 48  | 5     | 2093 | A    |
| 48  | 5     | 2094 | G    |
| 48  | 5     | 2095 | A    |
| 48  | 5     | 2097 | U    |
| 48  | 5     | 2100 | A    |
| 48  | 5     | 2101 | C    |
| 48  | 5     | 2103 | G    |
| 48  | 5     | 2107 | C    |
| 48  | 5     | 2108 | G    |
| 48  | 5     | 2109 | G    |
| 48  | 5     | 2110 | C    |
| 48  | 5     | 2111 | G    |
| 48  | 5     | 2112 | G    |
| 48  | 5     | 2113 | G    |
| 48  | 5     | 2114 | G    |
| 48  | 5     | 2115 | G    |
| 48  | 5     | 2116 | C    |
| 48  | 5     | 2117 | G    |
| 48  | 5     | 2118 | G    |
| 48  | 5     | 2119 | C    |
| 48  | 5     | 2120 | G    |
| 48  | 5     | 2122 | G    |
| 48  | 5     | 2123 | C    |
| 48  | 5     | 2124 | G    |
| 48  | 5     | 2125 | C    |
| 48  | 5     | 2126 | G    |
| 48  | 5     | 2127 | C    |
| 48  | 5     | 2129 | C    |
| 48  | 5     | 2130 | G    |
| 48  | 5     | 2131 | C    |
| 48  | 5     | 2247 | C    |
| 48  | 5     | 2248 | C    |
| 48  | 5     | 2250 | C    |
| 48  | 5     | 2251 | G    |
| 48  | 5     | 2252 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2253 | A    |
| 48  | 5     | 2254 | G    |
| 48  | 5     | 2255 | C    |
| 48  | 5     | 2256 | C    |
| 48  | 5     | 2257 | C    |
| 48  | 5     | 2258 | C    |
| 48  | 5     | 2259 | G    |
| 48  | 5     | 2260 | C    |
| 48  | 5     | 2261 | G    |
| 48  | 5     | 2263 | A    |
| 48  | 5     | 2264 | C    |
| 48  | 5     | 2265 | G    |
| 48  | 5     | 2266 | C    |
| 48  | 5     | 2267 | U    |
| 48  | 5     | 2268 | A    |
| 48  | 5     | 2269 | C    |
| 48  | 5     | 2270 | G    |
| 48  | 5     | 2274 | C    |
| 48  | 5     | 2275 | G    |
| 48  | 5     | 2279 | A    |
| 48  | 5     | 2288 | G    |
| 48  | 5     | 2289 | C    |
| 48  | 5     | 2299 | G    |
| 48  | 5     | 2300 | A    |
| 48  | 5     | 2301 | G    |
| 48  | 5     | 2312 | U    |
| 48  | 5     | 2313 | A    |
| 48  | 5     | 2314 | G    |
| 48  | 5     | 2324 | C    |
| 48  | 5     | 2331 | G    |
| 48  | 5     | 2332 | A    |
| 48  | 5     | 2333 | G    |
| 48  | 5     | 2335 | C    |
| 48  | 5     | 2337 | C    |
| 48  | 5     | 2348 | G    |
| 48  | 5     | 2351 | C    |
| 48  | 5     | 2360 | A    |
| 48  | 5     | 2364 | G    |
| 48  | 5     | 2370 | A    |
| 48  | 5     | 2382 | A    |
| 48  | 5     | 2383 | C    |
| 48  | 5     | 2395 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2396 | A    |
| 48  | 5     | 2399 | G    |
| 48  | 5     | 2417 | A    |
| 48  | 5     | 2422 | C    |
| 48  | 5     | 2424 | G    |
| 48  | 5     | 2425 | U    |
| 48  | 5     | 2428 | A    |
| 48  | 5     | 2429 | A    |
| 48  | 5     | 2433 | G    |
| 48  | 5     | 2434 | G    |
| 48  | 5     | 2440 | U    |
| 48  | 5     | 2441 | C    |
| 48  | 5     | 2447 | U    |
| 48  | 5     | 2450 | G    |
| 48  | 5     | 2458 | C    |
| 48  | 5     | 2469 | C    |
| 48  | 5     | 2471 | G    |
| 48  | 5     | 2473 | A    |
| 48  | 5     | 2474 | G    |
| 48  | 5     | 2475 | G    |
| 48  | 5     | 2485 | U    |
| 48  | 5     | 2488 | C    |
| 48  | 5     | 2489 | C    |
| 48  | 5     | 2490 | U    |
| 48  | 5     | 2491 | C    |
| 48  | 5     | 2493 | G    |
| 48  | 5     | 2495 | U    |
| 48  | 5     | 2499 | C    |
| 48  | 5     | 2503 | G    |
| 48  | 5     | 2504 | C    |
| 48  | 5     | 2505 | C    |
| 48  | 5     | 2506 | G    |
| 48  | 5     | 2507 | A    |
| 48  | 5     | 2512 | A    |
| 48  | 5     | 2513 | A    |
| 48  | 5     | 2514 | G    |
| 48  | 5     | 2519 | U    |
| 48  | 5     | 2521 | G    |
| 48  | 5     | 2527 | A    |
| 48  | 5     | 2530 | U    |
| 48  | 5     | 2536 | A    |
| 48  | 5     | 2537 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2544 | G    |
| 48  | 5     | 2546 | G    |
| 48  | 5     | 2547 | G    |
| 48  | 5     | 2553 | A    |
| 48  | 5     | 2554 | U    |
| 48  | 5     | 2555 | G    |
| 48  | 5     | 2564 | G    |
| 48  | 5     | 2566 | G    |
| 48  | 5     | 2568 | C    |
| 48  | 5     | 2571 | C    |
| 48  | 5     | 2575 | U    |
| 48  | 5     | 2577 | C    |
| 48  | 5     | 2583 | C    |
| 48  | 5     | 2587 | A    |
| 48  | 5     | 2588 | C    |
| 48  | 5     | 2589 | C    |
| 48  | 5     | 2591 | A    |
| 48  | 5     | 2601 | A    |
| 48  | 5     | 2602 | G    |
| 48  | 5     | 2611 | A    |
| 48  | 5     | 2620 | G    |
| 48  | 5     | 2623 | A    |
| 48  | 5     | 2627 | C    |
| 48  | 5     | 2638 | G    |
| 48  | 5     | 2640 | G    |
| 48  | 5     | 2647 | A    |
| 48  | 5     | 2653 | C    |
| 48  | 5     | 2661 | U    |
| 48  | 5     | 2662 | G    |
| 48  | 5     | 2663 | G    |
| 48  | 5     | 2669 | C    |
| 48  | 5     | 2673 | G    |
| 48  | 5     | 2676 | A    |
| 48  | 5     | 2679 | G    |
| 48  | 5     | 2681 | G    |
| 48  | 5     | 2686 | G    |
| 48  | 5     | 2687 | U    |
| 48  | 5     | 2688 | G    |
| 48  | 5     | 2695 | A    |
| 48  | 5     | 2696 | A    |
| 48  | 5     | 2704 | C    |
| 48  | 5     | 2708 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2710 | C    |
| 48  | 5     | 2711 | G    |
| 48  | 5     | 2712 | G    |
| 48  | 5     | 2714 | G    |
| 48  | 5     | 2716 | C    |
| 48  | 5     | 2721 | G    |
| 48  | 5     | 2724 | G    |
| 48  | 5     | 2725 | A    |
| 48  | 5     | 2726 | G    |
| 48  | 5     | 2733 | C    |
| 48  | 5     | 2740 | U    |
| 48  | 5     | 2743 | A    |
| 48  | 5     | 2754 | G    |
| 48  | 5     | 2755 | A    |
| 48  | 5     | 2756 | G    |
| 48  | 5     | 2760 | G    |
| 48  | 5     | 2761 | U    |
| 48  | 5     | 2762 | G    |
| 48  | 5     | 2767 | U    |
| 48  | 5     | 2768 | C    |
| 48  | 5     | 2769 | U    |
| 48  | 5     | 2770 | C    |
| 48  | 5     | 2772 | C    |
| 48  | 5     | 2787 | A    |
| 48  | 5     | 2788 | U    |
| 48  | 5     | 2789 | A    |
| 48  | 5     | 2790 | U    |
| 48  | 5     | 2794 | C    |
| 48  | 5     | 2795 | A    |
| 48  | 5     | 2796 | G    |
| 48  | 5     | 2798 | A    |
| 48  | 5     | 2806 | A    |
| 48  | 5     | 2807 | A    |
| 48  | 5     | 2814 | C    |
| 48  | 5     | 2824 | C    |
| 48  | 5     | 2825 | A    |
| 48  | 5     | 2826 | U    |
| 48  | 5     | 2827 | G    |
| 48  | 5     | 2828 | U    |
| 48  | 5     | 2829 | U    |
| 48  | 5     | 2835 | A    |
| 48  | 5     | 2838 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2839 | U    |
| 48  | 5     | 2842 | G    |
| 48  | 5     | 2855 | G    |
| 48  | 5     | 2859 | G    |
| 48  | 5     | 2862 | G    |
| 48  | 5     | 2869 | U    |
| 48  | 5     | 2896 | G    |
| 48  | 5     | 2897 | G    |
| 48  | 5     | 2898 | G    |
| 48  | 5     | 2904 | U    |
| 48  | 5     | 2905 | C    |
| 48  | 5     | 2910 | G    |
| 48  | 5     | 3594 | C    |
| 48  | 5     | 3595 | U    |
| 48  | 5     | 3596 | A    |
| 48  | 5     | 3597 | G    |
| 48  | 5     | 3598 | C    |
| 48  | 5     | 3605 | C    |
| 48  | 5     | 3606 | U    |
| 48  | 5     | 3615 | G    |
| 48  | 5     | 3617 | G    |
| 48  | 5     | 3625 | G    |
| 48  | 5     | 3626 | G    |
| 48  | 5     | 3630 | A    |
| 48  | 5     | 3635 | A    |
| 48  | 5     | 3644 | U    |
| 48  | 5     | 3653 | A    |
| 48  | 5     | 3662 | A    |
| 48  | 5     | 3668 | C    |
| 48  | 5     | 3670 | C    |
| 48  | 5     | 3671 | G    |
| 48  | 5     | 3673 | C    |
| 48  | 5     | 3674 | G    |
| 48  | 5     | 3680 | U    |
| 48  | 5     | 3682 | A    |
| 48  | 5     | 3689 | G    |
| 48  | 5     | 3692 | A    |
| 48  | 5     | 3696 | C    |
| 48  | 5     | 3698 | G    |
| 48  | 5     | 3702 | A    |
| 48  | 5     | 3709 | U    |
| 48  | 5     | 3710 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 3711 | A    |
| 48  | 5     | 3712 | A    |
| 48  | 5     | 3717 | A    |
| 48  | 5     | 3718 | A    |
| 48  | 5     | 3722 | G    |
| 48  | 5     | 3728 | A    |
| 48  | 5     | 3729 | U    |
| 48  | 5     | 3737 | A    |
| 48  | 5     | 3740 | G    |
| 48  | 5     | 3748 | A    |
| 48  | 5     | 3750 | G    |
| 48  | 5     | 3752 | C    |
| 48  | 5     | 3753 | G    |
| 48  | 5     | 3755 | G    |
| 48  | 5     | 3756 | A    |
| 48  | 5     | 3759 | A    |
| 48  | 5     | 3760 | A    |
| 48  | 5     | 3764 | U    |
| 48  | 5     | 3773 | U    |
| 48  | 5     | 3774 | A    |
| 48  | 5     | 3775 | A    |
| 48  | 5     | 3776 | G    |
| 48  | 5     | 3777 | G    |
| 48  | 5     | 3778 | U    |
| 48  | 5     | 3780 | G    |
| 48  | 5     | 3783 | A    |
| 48  | 5     | 3784 | A    |
| 48  | 5     | 3786 | U    |
| 48  | 5     | 3788 | C    |
| 48  | 5     | 3798 | U    |
| 48  | 5     | 3799 | A    |
| 48  | 5     | 3802 | U    |
| 48  | 5     | 3810 | C    |
| 48  | 5     | 3811 | G    |
| 48  | 5     | 3812 | C    |
| 48  | 5     | 3813 | A    |
| 48  | 5     | 3814 | U    |
| 48  | 5     | 3817 | A    |
| 48  | 5     | 3819 | G    |
| 48  | 5     | 3822 | U    |
| 48  | 5     | 3831 | U    |
| 48  | 5     | 3836 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 3838 | U    |
| 48  | 5     | 3839 | G    |
| 48  | 5     | 3840 | U    |
| 48  | 5     | 3859 | G    |
| 48  | 5     | 3867 | A    |
| 48  | 5     | 3877 | A    |
| 48  | 5     | 3878 | C    |
| 48  | 5     | 3879 | G    |
| 48  | 5     | 3889 | G    |
| 48  | 5     | 3897 | G    |
| 48  | 5     | 3900 | G    |
| 48  | 5     | 3901 | A    |
| 48  | 5     | 3905 | A    |
| 48  | 5     | 3906 | A    |
| 48  | 5     | 3907 | G    |
| 48  | 5     | 3912 | U    |
| 48  | 5     | 3915 | U    |
| 48  | 5     | 3916 | G    |
| 48  | 5     | 3917 | A    |
| 48  | 5     | 3924 | C    |
| 48  | 5     | 3925 | U    |
| 48  | 5     | 3926 | C    |
| 48  | 5     | 3927 | U    |
| 48  | 5     | 3938 | G    |
| 48  | 5     | 3939 | G    |
| 48  | 5     | 3943 | A    |
| 48  | 5     | 3946 | G    |
| 48  | 5     | 4069 | U    |
| 48  | 5     | 4070 | U    |
| 48  | 5     | 4076 | G    |
| 48  | 5     | 4084 | G    |
| 48  | 5     | 4085 | A    |
| 48  | 5     | 4086 | G    |
| 48  | 5     | 4087 | G    |
| 48  | 5     | 4088 | C    |
| 48  | 5     | 4091 | G    |
| 48  | 5     | 4092 | G    |
| 48  | 5     | 4093 | G    |
| 48  | 5     | 4094 | G    |
| 48  | 5     | 4097 | G    |
| 48  | 5     | 4104 | G    |
| 48  | 5     | 4105 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4107 | G    |
| 48  | 5     | 4112 | C    |
| 48  | 5     | 4114 | C    |
| 48  | 5     | 4115 | G    |
| 48  | 5     | 4116 | C    |
| 48  | 5     | 4117 | U    |
| 48  | 5     | 4118 | U    |
| 48  | 5     | 4119 | C    |
| 48  | 5     | 4120 | U    |
| 48  | 5     | 4121 | G    |
| 48  | 5     | 4122 | G    |
| 48  | 5     | 4125 | C    |
| 48  | 5     | 4127 | A    |
| 48  | 5     | 4134 | C    |
| 48  | 5     | 4143 | G    |
| 48  | 5     | 4144 | C    |
| 48  | 5     | 4145 | C    |
| 48  | 5     | 4155 | C    |
| 48  | 5     | 4161 | G    |
| 48  | 5     | 4162 | C    |
| 48  | 5     | 4163 | U    |
| 48  | 5     | 4165 | C    |
| 48  | 5     | 4166 | G    |
| 48  | 5     | 4168 | G    |
| 48  | 5     | 4170 | A    |
| 48  | 5     | 4171 | C    |
| 48  | 5     | 4182 | G    |
| 48  | 5     | 4183 | G    |
| 48  | 5     | 4184 | G    |
| 48  | 5     | 4191 | G    |
| 48  | 5     | 4203 | A    |
| 48  | 5     | 4208 | U    |
| 48  | 5     | 4212 | A    |
| 48  | 5     | 4213 | A    |
| 48  | 5     | 4216 | G    |
| 48  | 5     | 4217 | G    |
| 48  | 5     | 4218 | U    |
| 48  | 5     | 4219 | A    |
| 48  | 5     | 4225 | G    |
| 48  | 5     | 4226 | G    |
| 48  | 5     | 4229 | U    |
| 48  | 5     | 4232 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4233 | A    |
| 48  | 5     | 4238 | G    |
| 48  | 5     | 4241 | C    |
| 48  | 5     | 4251 | A    |
| 48  | 5     | 4254 | G    |
| 48  | 5     | 4258 | C    |
| 48  | 5     | 4265 | U    |
| 48  | 5     | 4266 | G    |
| 48  | 5     | 4267 | G    |
| 48  | 5     | 4268 | A    |
| 48  | 5     | 4271 | A    |
| 48  | 5     | 4273 | A    |
| 48  | 5     | 4282 | A    |
| 48  | 5     | 4291 | G    |
| 48  | 5     | 4297 | G    |
| 48  | 5     | 4302 | U    |
| 48  | 5     | 4303 | C    |
| 48  | 5     | 4304 | A    |
| 48  | 5     | 4305 | G    |
| 48  | 5     | 4306 | U    |
| 48  | 5     | 4307 | A    |
| 48  | 5     | 4311 | A    |
| 48  | 5     | 4312 | U    |
| 48  | 5     | 4313 | A    |
| 48  | 5     | 4314 | C    |
| 48  | 5     | 4317 | A    |
| 48  | 5     | 4318 | C    |
| 48  | 5     | 4319 | C    |
| 48  | 5     | 4329 | G    |
| 48  | 5     | 4330 | G    |
| 48  | 5     | 4331 | G    |
| 48  | 5     | 4332 | C    |
| 48  | 5     | 4335 | C    |
| 48  | 5     | 4336 | A    |
| 48  | 5     | 4349 | C    |
| 48  | 5     | 4350 | C    |
| 48  | 5     | 4354 | U    |
| 48  | 5     | 4355 | G    |
| 48  | 5     | 4360 | U    |
| 48  | 5     | 4367 | G    |
| 48  | 5     | 4368 | G    |
| 48  | 5     | 4372 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4373 | G    |
| 48  | 5     | 4377 | G    |
| 48  | 5     | 4378 | A    |
| 48  | 5     | 4379 | A    |
| 48  | 5     | 4380 | A    |
| 48  | 5     | 4387 | C    |
| 48  | 5     | 4391 | G    |
| 48  | 5     | 4394 | A    |
| 48  | 5     | 4395 | U    |
| 48  | 5     | 4396 | A    |
| 48  | 5     | 4398 | C    |
| 48  | 5     | 4405 | G    |
| 48  | 5     | 4419 | U    |
| 48  | 5     | 4420 | U    |
| 48  | 5     | 4421 | C    |
| 48  | 5     | 4422 | A    |
| 48  | 5     | 4424 | A    |
| 48  | 5     | 4426 | C    |
| 48  | 5     | 4430 | G    |
| 48  | 5     | 4433 | G    |
| 48  | 5     | 4438 | U    |
| 48  | 5     | 4439 | U    |
| 48  | 5     | 4441 | A    |
| 48  | 5     | 4444 | C    |
| 48  | 5     | 4448 | G    |
| 48  | 5     | 4449 | A    |
| 48  | 5     | 4450 | U    |
| 48  | 5     | 4453 | C    |
| 48  | 5     | 4454 | G    |
| 48  | 5     | 4464 | A    |
| 48  | 5     | 4471 | U    |
| 48  | 5     | 4472 | G    |
| 48  | 5     | 4473 | A    |
| 48  | 5     | 4475 | G    |
| 48  | 5     | 4476 | C    |
| 48  | 5     | 4481 | U    |
| 48  | 5     | 4482 | U    |
| 48  | 5     | 4484 | A    |
| 48  | 5     | 4488 | A    |
| 48  | 5     | 4491 | G    |
| 48  | 5     | 4495 | G    |
| 48  | 5     | 4500 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4510 | A    |
| 48  | 5     | 4511 | A    |
| 48  | 5     | 4512 | U    |
| 48  | 5     | 4513 | A    |
| 48  | 5     | 4515 | G    |
| 48  | 5     | 4519 | C    |
| 48  | 5     | 4520 | G    |
| 48  | 5     | 4522 | G    |
| 48  | 5     | 4524 | G    |
| 48  | 5     | 4527 | G    |
| 48  | 5     | 4528 | G    |
| 48  | 5     | 4529 | G    |
| 48  | 5     | 4535 | A    |
| 48  | 5     | 4548 | A    |
| 48  | 5     | 4549 | G    |
| 48  | 5     | 4550 | G    |
| 48  | 5     | 4557 | U    |
| 48  | 5     | 4567 | G    |
| 48  | 5     | 4570 | G    |
| 48  | 5     | 4573 | G    |
| 48  | 5     | 4575 | G    |
| 48  | 5     | 4577 | U    |
| 48  | 5     | 4583 | C    |
| 48  | 5     | 4584 | A    |
| 48  | 5     | 4585 | U    |
| 48  | 5     | 4586 | G    |
| 48  | 5     | 4590 | A    |
| 48  | 5     | 4591 | U    |
| 48  | 5     | 4606 | G    |
| 48  | 5     | 4618 | G    |
| 48  | 5     | 4636 | U    |
| 48  | 5     | 4637 | G    |
| 48  | 5     | 4641 | U    |
| 48  | 5     | 4647 | G    |
| 48  | 5     | 4648 | A    |
| 48  | 5     | 4656 | A    |
| 48  | 5     | 4657 | U    |
| 48  | 5     | 4661 | G    |
| 48  | 5     | 4670 | C    |
| 48  | 5     | 4672 | A    |
| 48  | 5     | 4677 | U    |
| 48  | 5     | 4687 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4694 | G    |
| 48  | 5     | 4695 | C    |
| 48  | 5     | 4700 | A    |
| 48  | 5     | 4701 | A    |
| 48  | 5     | 4702 | G    |
| 48  | 5     | 4709 | U    |
| 48  | 5     | 4719 | G    |
| 48  | 5     | 4720 | C    |
| 48  | 5     | 4721 | G    |
| 48  | 5     | 4730 | C    |
| 48  | 5     | 4731 | G    |
| 48  | 5     | 4732 | G    |
| 48  | 5     | 4733 | C    |
| 48  | 5     | 4734 | A    |
| 48  | 5     | 4737 | G    |
| 48  | 5     | 4741 | C    |
| 48  | 5     | 4745 | G    |
| 48  | 5     | 4746 | C    |
| 48  | 5     | 4749 | C    |
| 48  | 5     | 4750 | G    |
| 48  | 5     | 4753 | U    |
| 48  | 5     | 4754 | G    |
| 48  | 5     | 4756 | C    |
| 48  | 5     | 4758 | U    |
| 48  | 5     | 4760 | G    |
| 48  | 5     | 4764 | A    |
| 48  | 5     | 4768 | G    |
| 48  | 5     | 4770 | U    |
| 48  | 5     | 4771 | C    |
| 48  | 5     | 4774 | C    |
| 48  | 5     | 4869 | U    |
| 48  | 5     | 4871 | C    |
| 48  | 5     | 4872 | G    |
| 48  | 5     | 4873 | G    |
| 48  | 5     | 4874 | A    |
| 48  | 5     | 4875 | G    |
| 48  | 5     | 4876 | U    |
| 48  | 5     | 4877 | G    |
| 48  | 5     | 4878 | C    |
| 48  | 5     | 4883 | C    |
| 48  | 5     | 4884 | G    |
| 48  | 5     | 4885 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4886 | C    |
| 48  | 5     | 4889 | G    |
| 48  | 5     | 4890 | G    |
| 48  | 5     | 4893 | A    |
| 48  | 5     | 4895 | C    |
| 48  | 5     | 4896 | G    |
| 48  | 5     | 4898 | G    |
| 48  | 5     | 4900 | C    |
| 48  | 5     | 4901 | G    |
| 48  | 5     | 4904 | G    |
| 48  | 5     | 4906 | C    |
| 48  | 5     | 4910 | G    |
| 48  | 5     | 4911 | A    |
| 48  | 5     | 4912 | G    |
| 48  | 5     | 4913 | G    |
| 48  | 5     | 4924 | C    |
| 48  | 5     | 4926 | C    |
| 48  | 5     | 4927 | G    |
| 48  | 5     | 4930 | C    |
| 48  | 5     | 4931 | G    |
| 48  | 5     | 4932 | U    |
| 48  | 5     | 4934 | A    |
| 48  | 5     | 4935 | C    |
| 48  | 5     | 4936 | G    |
| 48  | 5     | 4939 | C    |
| 48  | 5     | 4942 | C    |
| 48  | 5     | 4945 | G    |
| 48  | 5     | 4948 | C    |
| 48  | 5     | 4949 | G    |
| 48  | 5     | 4950 | U    |
| 48  | 5     | 4951 | G    |
| 48  | 5     | 4952 | G    |
| 48  | 5     | 4959 | U    |
| 48  | 5     | 4964 | C    |
| 48  | 5     | 4965 | U    |
| 48  | 5     | 4966 | A    |
| 48  | 5     | 4967 | A    |
| 48  | 5     | 4975 | G    |
| 48  | 5     | 4976 | U    |
| 48  | 5     | 4985 | U    |
| 48  | 5     | 4988 | U    |
| 48  | 5     | 4989 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4990 | C    |
| 48  | 5     | 4991 | U    |
| 48  | 5     | 5007 | A    |
| 48  | 5     | 5013 | C    |
| 48  | 5     | 5014 | A    |
| 48  | 5     | 5017 | G    |
| 48  | 5     | 5018 | C    |
| 48  | 5     | 5022 | U    |
| 48  | 5     | 5023 | C    |
| 48  | 5     | 5024 | C    |
| 48  | 5     | 5025 | C    |
| 48  | 5     | 5026 | U    |
| 48  | 5     | 5027 | C    |
| 48  | 5     | 5028 | G    |
| 48  | 5     | 5031 | G    |
| 48  | 5     | 5033 | G    |
| 48  | 5     | 5041 | G    |
| 48  | 5     | 5047 | C    |
| 48  | 5     | 5050 | C    |
| 48  | 5     | 5052 | C    |
| 48  | 5     | 5053 | U    |
| 48  | 5     | 5054 | C    |
| 48  | 5     | 5056 | A    |
| 48  | 5     | 5058 | A    |
| 48  | 5     | 5060 | A    |
| 48  | 5     | 5061 | A    |
| 48  | 5     | 5062 | G    |
| 48  | 5     | 5066 | U    |
| 49  | 7     | 7    | G    |
| 49  | 7     | 11   | A    |
| 49  | 7     | 21   | G    |
| 49  | 7     | 25   | G    |
| 49  | 7     | 33   | U    |
| 49  | 7     | 40   | U    |
| 49  | 7     | 51   | G    |
| 49  | 7     | 53   | U    |
| 49  | 7     | 54   | A    |
| 49  | 7     | 64   | G    |
| 49  | 7     | 74   | A    |
| 49  | 7     | 76   | U    |
| 49  | 7     | 97   | G    |
| 49  | 7     | 99   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | 7     | 100 | A    |
| 49  | 7     | 106 | G    |
| 49  | 7     | 110 | G    |
| 49  | 7     | 111 | C    |
| 49  | 7     | 120 | U    |
| 50  | 8     | 2   | G    |
| 50  | 8     | 3   | A    |
| 50  | 8     | 34  | U    |
| 50  | 8     | 35  | C    |
| 50  | 8     | 38  | U    |
| 50  | 8     | 39  | G    |
| 50  | 8     | 49  | G    |
| 50  | 8     | 51  | U    |
| 50  | 8     | 52  | A    |
| 50  | 8     | 55  | U    |
| 50  | 8     | 57  | C    |
| 50  | 8     | 59  | A    |
| 50  | 8     | 62  | A    |
| 50  | 8     | 63  | U    |
| 50  | 8     | 74  | U    |
| 50  | 8     | 75  | G    |
| 50  | 8     | 79  | G    |
| 50  | 8     | 80  | A    |
| 50  | 8     | 81  | C    |
| 50  | 8     | 82  | A    |
| 50  | 8     | 83  | C    |
| 50  | 8     | 84  | A    |
| 50  | 8     | 85  | U    |
| 50  | 8     | 86  | U    |
| 50  | 8     | 87  | G    |
| 50  | 8     | 94  | G    |
| 50  | 8     | 95  | A    |
| 50  | 8     | 99  | U    |
| 50  | 8     | 101 | C    |
| 50  | 8     | 103 | A    |
| 50  | 8     | 104 | A    |
| 50  | 8     | 105 | C    |
| 50  | 8     | 107 | C    |
| 50  | 8     | 109 | C    |
| 50  | 8     | 110 | U    |
| 50  | 8     | 111 | U    |
| 50  | 8     | 112 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | 8     | 113 | C    |
| 50  | 8     | 114 | G    |
| 50  | 8     | 115 | G    |
| 50  | 8     | 117 | C    |
| 50  | 8     | 121 | G    |
| 50  | 8     | 122 | G    |
| 50  | 8     | 123 | U    |
| 50  | 8     | 124 | U    |
| 50  | 8     | 125 | C    |
| 50  | 8     | 126 | C    |
| 50  | 8     | 127 | U    |
| 50  | 8     | 137 | A    |
| 50  | 8     | 143 | G    |
| 50  | 8     | 150 | C    |
| 50  | 8     | 156 | U    |
| 51  | 9     | 2   | A    |
| 51  | 9     | 3   | C    |
| 51  | 9     | 4   | C    |
| 51  | 9     | 6   | G    |
| 51  | 9     | 9   | U    |
| 51  | 9     | 10  | G    |
| 51  | 9     | 11  | A    |
| 51  | 9     | 17  | C    |
| 51  | 9     | 19  | A    |
| 51  | 9     | 25  | A    |
| 51  | 9     | 26  | U    |
| 51  | 9     | 33  | G    |
| 51  | 9     | 37  | C    |
| 51  | 9     | 41  | G    |
| 51  | 9     | 42  | A    |
| 51  | 9     | 44  | U    |
| 51  | 9     | 45  | A    |
| 51  | 9     | 46  | A    |
| 51  | 9     | 49  | C    |
| 51  | 9     | 56  | G    |
| 51  | 9     | 58  | C    |
| 51  | 9     | 59  | U    |
| 51  | 9     | 60  | A    |
| 51  | 9     | 61  | A    |
| 51  | 9     | 63  | U    |
| 51  | 9     | 65  | C    |
| 51  | 9     | 66  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 67  | C    |
| 51  | 9     | 68  | A    |
| 51  | 9     | 70  | G    |
| 51  | 9     | 71  | G    |
| 51  | 9     | 72  | C    |
| 51  | 9     | 73  | C    |
| 51  | 9     | 74  | G    |
| 51  | 9     | 75  | G    |
| 51  | 9     | 76  | U    |
| 51  | 9     | 77  | A    |
| 51  | 9     | 78  | C    |
| 51  | 9     | 79  | A    |
| 51  | 9     | 80  | G    |
| 51  | 9     | 93  | U    |
| 51  | 9     | 95  | G    |
| 51  | 9     | 99  | A    |
| 51  | 9     | 100 | U    |
| 51  | 9     | 103 | A    |
| 51  | 9     | 109 | U    |
| 51  | 9     | 110 | U    |
| 51  | 9     | 111 | A    |
| 51  | 9     | 113 | G    |
| 51  | 9     | 114 | G    |
| 51  | 9     | 115 | U    |
| 51  | 9     | 116 | U    |
| 51  | 9     | 119 | U    |
| 51  | 9     | 124 | U    |
| 51  | 9     | 126 | G    |
| 51  | 9     | 140 | C    |
| 51  | 9     | 141 | A    |
| 51  | 9     | 142 | C    |
| 51  | 9     | 147 | A    |
| 51  | 9     | 150 | A    |
| 51  | 9     | 155 | G    |
| 51  | 9     | 158 | A    |
| 51  | 9     | 161 | U    |
| 51  | 9     | 162 | C    |
| 51  | 9     | 163 | U    |
| 51  | 9     | 164 | A    |
| 51  | 9     | 165 | G    |
| 51  | 9     | 167 | G    |
| 51  | 9     | 168 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 173 | A    |
| 51  | 9     | 180 | G    |
| 51  | 9     | 183 | G    |
| 51  | 9     | 184 | G    |
| 51  | 9     | 185 | G    |
| 51  | 9     | 188 | C    |
| 51  | 9     | 189 | U    |
| 51  | 9     | 190 | G    |
| 51  | 9     | 191 | A    |
| 51  | 9     | 192 | C    |
| 51  | 9     | 202 | G    |
| 51  | 9     | 206 | G    |
| 51  | 9     | 213 | G    |
| 51  | 9     | 215 | G    |
| 51  | 9     | 216 | C    |
| 51  | 9     | 225 | G    |
| 51  | 9     | 289 | G    |
| 51  | 9     | 291 | G    |
| 51  | 9     | 292 | A    |
| 51  | 9     | 293 | C    |
| 51  | 9     | 294 | U    |
| 51  | 9     | 302 | A    |
| 51  | 9     | 304 | C    |
| 51  | 9     | 305 | U    |
| 51  | 9     | 306 | C    |
| 51  | 9     | 307 | G    |
| 51  | 9     | 308 | G    |
| 51  | 9     | 309 | G    |
| 51  | 9     | 310 | C    |
| 51  | 9     | 312 | G    |
| 51  | 9     | 313 | A    |
| 51  | 9     | 314 | U    |
| 51  | 9     | 320 | G    |
| 51  | 9     | 321 | C    |
| 51  | 9     | 322 | C    |
| 51  | 9     | 323 | C    |
| 51  | 9     | 324 | C    |
| 51  | 9     | 326 | C    |
| 51  | 9     | 327 | G    |
| 51  | 9     | 328 | U    |
| 51  | 9     | 338 | G    |
| 51  | 9     | 339 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 343 | A    |
| 51  | 9     | 347 | G    |
| 51  | 9     | 350 | C    |
| 51  | 9     | 351 | G    |
| 51  | 9     | 355 | G    |
| 51  | 9     | 360 | A    |
| 51  | 9     | 362 | C    |
| 51  | 9     | 364 | A    |
| 51  | 9     | 368 | U    |
| 51  | 9     | 370 | G    |
| 51  | 9     | 373 | G    |
| 51  | 9     | 385 | G    |
| 51  | 9     | 386 | C    |
| 51  | 9     | 400 | C    |
| 51  | 9     | 407 | G    |
| 51  | 9     | 408 | A    |
| 51  | 9     | 409 | C    |
| 51  | 9     | 416 | U    |
| 51  | 9     | 417 | C    |
| 51  | 9     | 418 | A    |
| 51  | 9     | 428 | U    |
| 51  | 9     | 432 | G    |
| 51  | 9     | 435 | A    |
| 51  | 9     | 438 | G    |
| 51  | 9     | 441 | C    |
| 51  | 9     | 447 | A    |
| 51  | 9     | 448 | A    |
| 51  | 9     | 449 | A    |
| 51  | 9     | 450 | C    |
| 51  | 9     | 457 | C    |
| 51  | 9     | 459 | C    |
| 51  | 9     | 460 | A    |
| 51  | 9     | 464 | A    |
| 51  | 9     | 465 | A    |
| 51  | 9     | 466 | G    |
| 51  | 9     | 467 | G    |
| 51  | 9     | 469 | A    |
| 51  | 9     | 472 | C    |
| 51  | 9     | 473 | A    |
| 51  | 9     | 474 | G    |
| 51  | 9     | 482 | G    |
| 51  | 9     | 483 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 487 | U    |
| 51  | 9     | 488 | U    |
| 51  | 9     | 489 | A    |
| 51  | 9     | 492 | C    |
| 51  | 9     | 493 | A    |
| 51  | 9     | 503 | C    |
| 51  | 9     | 508 | A    |
| 51  | 9     | 511 | U    |
| 51  | 9     | 512 | A    |
| 51  | 9     | 523 | A    |
| 51  | 9     | 525 | A    |
| 51  | 9     | 528 | A    |
| 51  | 9     | 530 | U    |
| 51  | 9     | 532 | C    |
| 51  | 9     | 533 | A    |
| 51  | 9     | 535 | G    |
| 51  | 9     | 539 | C    |
| 51  | 9     | 544 | G    |
| 51  | 9     | 545 | A    |
| 51  | 9     | 546 | G    |
| 51  | 9     | 548 | C    |
| 51  | 9     | 549 | C    |
| 51  | 9     | 550 | C    |
| 51  | 9     | 551 | U    |
| 51  | 9     | 552 | G    |
| 51  | 9     | 554 | A    |
| 51  | 9     | 556 | U    |
| 51  | 9     | 557 | U    |
| 51  | 9     | 559 | G    |
| 51  | 9     | 560 | A    |
| 51  | 9     | 562 | U    |
| 51  | 9     | 563 | G    |
| 51  | 9     | 568 | C    |
| 51  | 9     | 576 | A    |
| 51  | 9     | 577 | U    |
| 51  | 9     | 579 | C    |
| 51  | 9     | 583 | A    |
| 51  | 9     | 587 | A    |
| 51  | 9     | 588 | G    |
| 51  | 9     | 589 | G    |
| 51  | 9     | 590 | A    |
| 51  | 9     | 591 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 592 | C    |
| 51  | 9     | 593 | C    |
| 51  | 9     | 594 | A    |
| 51  | 9     | 595 | U    |
| 51  | 9     | 596 | U    |
| 51  | 9     | 597 | G    |
| 51  | 9     | 598 | G    |
| 51  | 9     | 603 | C    |
| 51  | 9     | 604 | A    |
| 51  | 9     | 605 | A    |
| 51  | 9     | 606 | G    |
| 51  | 9     | 607 | U    |
| 51  | 9     | 608 | C    |
| 51  | 9     | 609 | U    |
| 51  | 9     | 613 | G    |
| 51  | 9     | 614 | C    |
| 51  | 9     | 620 | G    |
| 51  | 9     | 621 | C    |
| 51  | 9     | 623 | G    |
| 51  | 9     | 627 | U    |
| 51  | 9     | 628 | A    |
| 51  | 9     | 629 | A    |
| 51  | 9     | 631 | U    |
| 51  | 9     | 632 | C    |
| 51  | 9     | 643 | A    |
| 51  | 9     | 644 | G    |
| 51  | 9     | 654 | A    |
| 51  | 9     | 658 | U    |
| 51  | 9     | 659 | G    |
| 51  | 9     | 660 | C    |
| 51  | 9     | 663 | C    |
| 51  | 9     | 664 | A    |
| 51  | 9     | 668 | A    |
| 51  | 9     | 669 | A    |
| 51  | 9     | 671 | A    |
| 51  | 9     | 672 | A    |
| 51  | 9     | 673 | G    |
| 51  | 9     | 684 | G    |
| 51  | 9     | 688 | U    |
| 51  | 9     | 689 | U    |
| 51  | 9     | 698 | G    |
| 51  | 9     | 731 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 735 | C    |
| 51  | 9     | 737 | G    |
| 51  | 9     | 738 | C    |
| 51  | 9     | 747 | U    |
| 51  | 9     | 748 | C    |
| 51  | 9     | 749 | U    |
| 51  | 9     | 752 | G    |
| 51  | 9     | 753 | C    |
| 51  | 9     | 788 | G    |
| 51  | 9     | 791 | C    |
| 51  | 9     | 794 | A    |
| 51  | 9     | 796 | G    |
| 51  | 9     | 797 | C    |
| 51  | 9     | 798 | G    |
| 51  | 9     | 799 | U    |
| 51  | 9     | 800 | U    |
| 51  | 9     | 810 | A    |
| 51  | 9     | 811 | A    |
| 51  | 9     | 812 | A    |
| 51  | 9     | 821 | G    |
| 51  | 9     | 822 | U    |
| 51  | 9     | 830 | A    |
| 51  | 9     | 833 | C    |
| 51  | 9     | 834 | C    |
| 51  | 9     | 835 | C    |
| 51  | 9     | 836 | G    |
| 51  | 9     | 837 | A    |
| 51  | 9     | 838 | G    |
| 51  | 9     | 839 | C    |
| 51  | 9     | 840 | C    |
| 51  | 9     | 844 | U    |
| 51  | 9     | 845 | G    |
| 51  | 9     | 847 | A    |
| 51  | 9     | 859 | G    |
| 51  | 9     | 869 | A    |
| 51  | 9     | 870 | A    |
| 51  | 9     | 871 | U    |
| 51  | 9     | 872 | A    |
| 51  | 9     | 873 | G    |
| 51  | 9     | 875 | A    |
| 51  | 9     | 877 | C    |
| 51  | 9     | 878 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 879  | C    |
| 51  | 9     | 880  | G    |
| 51  | 9     | 887  | U    |
| 51  | 9     | 888  | U    |
| 51  | 9     | 890  | U    |
| 51  | 9     | 892  | U    |
| 51  | 9     | 893  | U    |
| 51  | 9     | 901  | G    |
| 51  | 9     | 902  | G    |
| 51  | 9     | 903  | A    |
| 51  | 9     | 909  | G    |
| 51  | 9     | 910  | G    |
| 51  | 9     | 912  | C    |
| 51  | 9     | 913  | A    |
| 51  | 9     | 914  | U    |
| 51  | 9     | 917  | U    |
| 51  | 9     | 919  | A    |
| 51  | 9     | 920  | A    |
| 51  | 9     | 921  | G    |
| 51  | 9     | 922  | A    |
| 51  | 9     | 930  | C    |
| 51  | 9     | 933  | G    |
| 51  | 9     | 934  | G    |
| 51  | 9     | 938  | A    |
| 51  | 9     | 943  | U    |
| 51  | 9     | 956  | G    |
| 51  | 9     | 958  | G    |
| 51  | 9     | 971  | G    |
| 51  | 9     | 978  | G    |
| 51  | 9     | 985  | G    |
| 51  | 9     | 990  | A    |
| 51  | 9     | 992  | A    |
| 51  | 9     | 996  | A    |
| 51  | 9     | 999  | G    |
| 51  | 9     | 1002 | U    |
| 51  | 9     | 1016 | U    |
| 51  | 9     | 1017 | U    |
| 51  | 9     | 1023 | A    |
| 51  | 9     | 1033 | G    |
| 51  | 9     | 1040 | G    |
| 51  | 9     | 1041 | G    |
| 51  | 9     | 1044 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1045 | U    |
| 51  | 9     | 1049 | A    |
| 51  | 9     | 1058 | A    |
| 51  | 9     | 1060 | A    |
| 51  | 9     | 1083 | A    |
| 51  | 9     | 1085 | C    |
| 51  | 9     | 1089 | G    |
| 51  | 9     | 1096 | G    |
| 51  | 9     | 1099 | G    |
| 51  | 9     | 1100 | A    |
| 51  | 9     | 1109 | C    |
| 51  | 9     | 1110 | G    |
| 51  | 9     | 1111 | U    |
| 51  | 9     | 1113 | A    |
| 51  | 9     | 1114 | U    |
| 51  | 9     | 1115 | U    |
| 51  | 9     | 1116 | C    |
| 51  | 9     | 1117 | C    |
| 51  | 9     | 1118 | C    |
| 51  | 9     | 1120 | U    |
| 51  | 9     | 1121 | G    |
| 51  | 9     | 1126 | G    |
| 51  | 9     | 1131 | G    |
| 51  | 9     | 1133 | A    |
| 51  | 9     | 1137 | U    |
| 51  | 9     | 1138 | C    |
| 51  | 9     | 1139 | C    |
| 51  | 9     | 1143 | A    |
| 51  | 9     | 1144 | A    |
| 51  | 9     | 1146 | C    |
| 51  | 9     | 1148 | A    |
| 51  | 9     | 1149 | A    |
| 51  | 9     | 1150 | A    |
| 51  | 9     | 1153 | C    |
| 51  | 9     | 1154 | U    |
| 51  | 9     | 1161 | U    |
| 51  | 9     | 1165 | G    |
| 51  | 9     | 1166 | G    |
| 51  | 9     | 1170 | A    |
| 51  | 9     | 1181 | A    |
| 51  | 9     | 1195 | A    |
| 51  | 9     | 1207 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1208 | A    |
| 51  | 9     | 1209 | A    |
| 51  | 9     | 1211 | G    |
| 51  | 9     | 1212 | G    |
| 51  | 9     | 1213 | C    |
| 51  | 9     | 1215 | C    |
| 51  | 9     | 1221 | G    |
| 51  | 9     | 1224 | G    |
| 51  | 9     | 1227 | G    |
| 51  | 9     | 1240 | A    |
| 51  | 9     | 1242 | U    |
| 51  | 9     | 1243 | U    |
| 51  | 9     | 1244 | U    |
| 51  | 9     | 1247 | C    |
| 51  | 9     | 1248 | U    |
| 51  | 9     | 1250 | A    |
| 51  | 9     | 1251 | A    |
| 51  | 9     | 1253 | A    |
| 51  | 9     | 1254 | C    |
| 51  | 9     | 1256 | G    |
| 51  | 9     | 1257 | G    |
| 51  | 9     | 1258 | A    |
| 51  | 9     | 1259 | A    |
| 51  | 9     | 1265 | A    |
| 51  | 9     | 1266 | C    |
| 51  | 9     | 1267 | C    |
| 51  | 9     | 1268 | C    |
| 51  | 9     | 1270 | G    |
| 51  | 9     | 1271 | C    |
| 51  | 9     | 1274 | G    |
| 51  | 9     | 1275 | G    |
| 51  | 9     | 1276 | A    |
| 51  | 9     | 1280 | G    |
| 51  | 9     | 1283 | C    |
| 51  | 9     | 1284 | A    |
| 51  | 9     | 1285 | G    |
| 51  | 9     | 1286 | G    |
| 51  | 9     | 1288 | U    |
| 51  | 9     | 1289 | U    |
| 51  | 9     | 1291 | A    |
| 51  | 9     | 1292 | C    |
| 51  | 9     | 1293 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1294 | G    |
| 51  | 9     | 1295 | A    |
| 51  | 9     | 1299 | A    |
| 51  | 9     | 1301 | A    |
| 51  | 9     | 1302 | G    |
| 51  | 9     | 1303 | C    |
| 51  | 9     | 1308 | U    |
| 51  | 9     | 1309 | C    |
| 51  | 9     | 1310 | U    |
| 51  | 9     | 1312 | G    |
| 51  | 9     | 1314 | U    |
| 51  | 9     | 1315 | U    |
| 51  | 9     | 1316 | C    |
| 51  | 9     | 1322 | G    |
| 51  | 9     | 1330 | G    |
| 51  | 9     | 1331 | C    |
| 51  | 9     | 1342 | U    |
| 51  | 9     | 1343 | U    |
| 51  | 9     | 1345 | G    |
| 51  | 9     | 1347 | U    |
| 51  | 9     | 1348 | G    |
| 51  | 9     | 1364 | U    |
| 51  | 9     | 1371 | U    |
| 51  | 9     | 1372 | U    |
| 51  | 9     | 1378 | A    |
| 51  | 9     | 1386 | A    |
| 51  | 9     | 1394 | G    |
| 51  | 9     | 1395 | C    |
| 51  | 9     | 1396 | A    |
| 51  | 9     | 1397 | U    |
| 51  | 9     | 1398 | G    |
| 51  | 9     | 1401 | A    |
| 51  | 9     | 1402 | A    |
| 51  | 9     | 1403 | C    |
| 51  | 9     | 1404 | U    |
| 51  | 9     | 1405 | A    |
| 51  | 9     | 1407 | U    |
| 51  | 9     | 1408 | U    |
| 51  | 9     | 1410 | C    |
| 51  | 9     | 1412 | C    |
| 51  | 9     | 1413 | G    |
| 51  | 9     | 1414 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1417 | C    |
| 51  | 9     | 1418 | C    |
| 51  | 9     | 1419 | C    |
| 51  | 9     | 1420 | G    |
| 51  | 9     | 1422 | G    |
| 51  | 9     | 1424 | G    |
| 51  | 9     | 1426 | U    |
| 51  | 9     | 1427 | C    |
| 51  | 9     | 1432 | U    |
| 51  | 9     | 1433 | C    |
| 51  | 9     | 1434 | C    |
| 51  | 9     | 1437 | C    |
| 51  | 9     | 1438 | A    |
| 51  | 9     | 1439 | A    |
| 51  | 9     | 1440 | C    |
| 51  | 9     | 1442 | U    |
| 51  | 9     | 1447 | G    |
| 51  | 9     | 1448 | A    |
| 51  | 9     | 1449 | G    |
| 51  | 9     | 1450 | G    |
| 51  | 9     | 1452 | A    |
| 51  | 9     | 1454 | A    |
| 51  | 9     | 1455 | A    |
| 51  | 9     | 1456 | G    |
| 51  | 9     | 1459 | G    |
| 51  | 9     | 1462 | U    |
| 51  | 9     | 1463 | U    |
| 51  | 9     | 1464 | C    |
| 51  | 9     | 1466 | G    |
| 51  | 9     | 1473 | G    |
| 51  | 9     | 1474 | A    |
| 51  | 9     | 1475 | G    |
| 51  | 9     | 1476 | A    |
| 51  | 9     | 1477 | U    |
| 51  | 9     | 1478 | U    |
| 51  | 9     | 1489 | A    |
| 51  | 9     | 1490 | G    |
| 51  | 9     | 1494 | U    |
| 51  | 9     | 1495 | G    |
| 51  | 9     | 1496 | U    |
| 51  | 9     | 1498 | A    |
| 51  | 9     | 1499 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1500 | G    |
| 51  | 9     | 1507 | G    |
| 51  | 9     | 1510 | G    |
| 51  | 9     | 1521 | C    |
| 51  | 9     | 1522 | A    |
| 51  | 9     | 1523 | C    |
| 51  | 9     | 1525 | C    |
| 51  | 9     | 1531 | A    |
| 51  | 9     | 1533 | A    |
| 51  | 9     | 1535 | U    |
| 51  | 9     | 1536 | G    |
| 51  | 9     | 1544 | C    |
| 51  | 9     | 1545 | A    |
| 51  | 9     | 1548 | G    |
| 51  | 9     | 1552 | G    |
| 51  | 9     | 1553 | C    |
| 51  | 9     | 1554 | C    |
| 51  | 9     | 1555 | U    |
| 51  | 9     | 1556 | A    |
| 51  | 9     | 1558 | C    |
| 51  | 9     | 1560 | U    |
| 51  | 9     | 1563 | G    |
| 51  | 9     | 1564 | C    |
| 51  | 9     | 1565 | C    |
| 51  | 9     | 1567 | G    |
| 51  | 9     | 1570 | G    |
| 51  | 9     | 1574 | C    |
| 51  | 9     | 1575 | G    |
| 51  | 9     | 1580 | A    |
| 51  | 9     | 1581 | C    |
| 51  | 9     | 1582 | C    |
| 51  | 9     | 1585 | U    |
| 51  | 9     | 1586 | U    |
| 51  | 9     | 1587 | G    |
| 51  | 9     | 1588 | A    |
| 51  | 9     | 1589 | A    |
| 51  | 9     | 1594 | A    |
| 51  | 9     | 1595 | U    |
| 51  | 9     | 1596 | U    |
| 51  | 9     | 1599 | U    |
| 51  | 9     | 1600 | G    |
| 51  | 9     | 1601 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1603 | G    |
| 51  | 9     | 1604 | G    |
| 51  | 9     | 1606 | G    |
| 51  | 9     | 1618 | C    |
| 51  | 9     | 1621 | U    |
| 51  | 9     | 1622 | U    |
| 51  | 9     | 1623 | A    |
| 51  | 9     | 1624 | U    |
| 51  | 9     | 1625 | U    |
| 51  | 9     | 1630 | A    |
| 51  | 9     | 1632 | G    |
| 51  | 9     | 1633 | A    |
| 51  | 9     | 1637 | A    |
| 51  | 9     | 1638 | G    |
| 51  | 9     | 1639 | G    |
| 51  | 9     | 1641 | A    |
| 51  | 9     | 1647 | A    |
| 51  | 9     | 1648 | G    |
| 51  | 9     | 1654 | G    |
| 51  | 9     | 1664 | A    |
| 51  | 9     | 1665 | G    |
| 51  | 9     | 1671 | G    |
| 51  | 9     | 1672 | U    |
| 51  | 9     | 1680 | G    |
| 51  | 9     | 1681 | U    |
| 51  | 9     | 1682 | C    |
| 51  | 9     | 1683 | C    |
| 51  | 9     | 1686 | G    |
| 51  | 9     | 1688 | C    |
| 51  | 9     | 1689 | C    |
| 51  | 9     | 1695 | A    |
| 51  | 9     | 1698 | C    |
| 51  | 9     | 1699 | A    |
| 51  | 9     | 1706 | G    |
| 51  | 9     | 1715 | A    |
| 51  | 9     | 1721 | U    |
| 51  | 9     | 1722 | G    |
| 51  | 9     | 1725 | U    |
| 51  | 9     | 1728 | U    |
| 51  | 9     | 1729 | U    |
| 51  | 9     | 1739 | C    |
| 51  | 9     | 1742 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1745 | A    |
| 51  | 9     | 1746 | U    |
| 51  | 9     | 1750 | C    |
| 51  | 9     | 1753 | C    |
| 51  | 9     | 1756 | C    |
| 51  | 9     | 1757 | G    |
| 51  | 9     | 1758 | G    |
| 51  | 9     | 1783 | C    |
| 51  | 9     | 1786 | U    |
| 51  | 9     | 1789 | G    |
| 51  | 9     | 1800 | A    |
| 51  | 9     | 1802 | C    |
| 51  | 9     | 1809 | A    |
| 51  | 9     | 1812 | U    |
| 51  | 9     | 1813 | A    |
| 51  | 9     | 1823 | A    |
| 51  | 9     | 1824 | A    |
| 51  | 9     | 1825 | A    |
| 51  | 9     | 1826 | G    |
| 51  | 9     | 1827 | U    |
| 51  | 9     | 1829 | G    |
| 51  | 9     | 1831 | A    |
| 51  | 9     | 1835 | A    |
| 51  | 9     | 1836 | G    |
| 51  | 9     | 1837 | G    |
| 51  | 9     | 1838 | U    |
| 51  | 9     | 1839 | U    |
| 51  | 9     | 1849 | G    |
| 51  | 9     | 1850 | A    |
| 51  | 9     | 1851 | A    |
| 51  | 9     | 1861 | G    |
| 51  | 9     | 1862 | G    |
| 51  | 9     | 1863 | A    |
| 51  | 9     | 1865 | C    |
| 51  | 9     | 1867 | U    |
| 85  | hh    | 42   | C    |
| 85  | hh    | 43   | A    |
| 85  | hh    | 45   | A    |
| 85  | hh    | 46   | G    |
| 85  | hh    | 49   | U    |
| 85  | hh    | 50   | A    |
| 85  | hh    | 52   | G    |

All (413) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | 2     | 34  | A    |
| 47  | 3     | 7   | A    |
| 47  | 3     | 9   | A    |
| 47  | 3     | 29  | A    |
| 47  | 3     | 30  | G    |
| 47  | 3     | 60  | U    |
| 47  | 3     | 69  | G    |
| 47  | 3     | 74  | C    |
| 48  | 5     | 1   | C    |
| 48  | 5     | 12  | A    |
| 48  | 5     | 20  | U    |
| 48  | 5     | 39  | A    |
| 48  | 5     | 42  | A    |
| 48  | 5     | 47  | A    |
| 48  | 5     | 48  | G    |
| 48  | 5     | 58  | G    |
| 48  | 5     | 64  | A    |
| 48  | 5     | 72  | C    |
| 48  | 5     | 90  | G    |
| 48  | 5     | 93  | G    |
| 48  | 5     | 119 | G    |
| 48  | 5     | 120 | A    |
| 48  | 5     | 125 | C    |
| 48  | 5     | 126 | C    |
| 48  | 5     | 134 | G    |
| 48  | 5     | 143 | C    |
| 48  | 5     | 157 | U    |
| 48  | 5     | 159 | C    |
| 48  | 5     | 170 | C    |
| 48  | 5     | 187 | U    |
| 48  | 5     | 215 | C    |
| 48  | 5     | 216 | C    |
| 48  | 5     | 218 | A    |
| 48  | 5     | 219 | G    |
| 48  | 5     | 224 | U    |
| 48  | 5     | 226 | G    |
| 48  | 5     | 245 | C    |
| 48  | 5     | 253 | G    |
| 48  | 5     | 265 | C    |
| 48  | 5     | 266 | C    |
| 48  | 5     | 275 | C    |
| 48  | 5     | 286 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 296  | A    |
| 48  | 5     | 361  | C    |
| 48  | 5     | 385  | A    |
| 48  | 5     | 387  | G    |
| 48  | 5     | 406  | C    |
| 48  | 5     | 451  | C    |
| 48  | 5     | 454  | U    |
| 48  | 5     | 486  | C    |
| 48  | 5     | 497  | G    |
| 48  | 5     | 505  | G    |
| 48  | 5     | 509  | A    |
| 48  | 5     | 664  | G    |
| 48  | 5     | 684  | G    |
| 48  | 5     | 693  | C    |
| 48  | 5     | 727  | C    |
| 48  | 5     | 728  | U    |
| 48  | 5     | 733  | A    |
| 48  | 5     | 746  | A    |
| 48  | 5     | 747  | A    |
| 48  | 5     | 917  | A    |
| 48  | 5     | 930  | G    |
| 48  | 5     | 931  | C    |
| 48  | 5     | 932  | A    |
| 48  | 5     | 935  | A    |
| 48  | 5     | 943  | A    |
| 48  | 5     | 956  | A    |
| 48  | 5     | 957  | G    |
| 48  | 5     | 965  | G    |
| 48  | 5     | 977  | C    |
| 48  | 5     | 978  | G    |
| 48  | 5     | 989  | U    |
| 48  | 5     | 1071 | C    |
| 48  | 5     | 1176 | C    |
| 48  | 5     | 1211 | G    |
| 48  | 5     | 1214 | C    |
| 48  | 5     | 1232 | G    |
| 48  | 5     | 1236 | C    |
| 48  | 5     | 1237 | C    |
| 48  | 5     | 1238 | A    |
| 48  | 5     | 1239 | C    |
| 48  | 5     | 1241 | C    |
| 48  | 5     | 1266 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1268 | G    |
| 48  | 5     | 1272 | C    |
| 48  | 5     | 1279 | A    |
| 48  | 5     | 1280 | C    |
| 48  | 5     | 1292 | C    |
| 48  | 5     | 1296 | G    |
| 48  | 5     | 1329 | G    |
| 48  | 5     | 1354 | A    |
| 48  | 5     | 1357 | C    |
| 48  | 5     | 1365 | C    |
| 48  | 5     | 1370 | G    |
| 48  | 5     | 1371 | A    |
| 48  | 5     | 1376 | C    |
| 48  | 5     | 1379 | C    |
| 48  | 5     | 1380 | G    |
| 48  | 5     | 1390 | G    |
| 48  | 5     | 1398 | A    |
| 48  | 5     | 1407 | C    |
| 48  | 5     | 1410 | U    |
| 48  | 5     | 1419 | G    |
| 48  | 5     | 1420 | A    |
| 48  | 5     | 1435 | G    |
| 48  | 5     | 1440 | U    |
| 48  | 5     | 1445 | U    |
| 48  | 5     | 1455 | G    |
| 48  | 5     | 1474 | C    |
| 48  | 5     | 1477 | C    |
| 48  | 5     | 1481 | C    |
| 48  | 5     | 1485 | C    |
| 48  | 5     | 1500 | A    |
| 48  | 5     | 1523 | A    |
| 48  | 5     | 1533 | A    |
| 48  | 5     | 1563 | A    |
| 48  | 5     | 1625 | G    |
| 48  | 5     | 1633 | G    |
| 48  | 5     | 1654 | G    |
| 48  | 5     | 1678 | C    |
| 48  | 5     | 1696 | C    |
| 48  | 5     | 1697 | G    |
| 48  | 5     | 1724 | G    |
| 48  | 5     | 1733 | G    |
| 48  | 5     | 1741 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 1755 | C    |
| 48  | 5     | 1756 | U    |
| 48  | 5     | 1804 | A    |
| 48  | 5     | 1818 | G    |
| 48  | 5     | 1819 | G    |
| 48  | 5     | 1835 | G    |
| 48  | 5     | 1839 | U    |
| 48  | 5     | 1891 | A    |
| 48  | 5     | 1892 | A    |
| 48  | 5     | 1921 | C    |
| 48  | 5     | 1935 | C    |
| 48  | 5     | 1956 | A    |
| 48  | 5     | 1957 | U    |
| 48  | 5     | 1958 | A    |
| 48  | 5     | 1959 | U    |
| 48  | 5     | 1960 | A    |
| 48  | 5     | 1961 | G    |
| 48  | 5     | 1968 | G    |
| 48  | 5     | 1969 | G    |
| 48  | 5     | 1974 | U    |
| 48  | 5     | 1975 | G    |
| 48  | 5     | 1986 | U    |
| 48  | 5     | 2009 | A    |
| 48  | 5     | 2019 | C    |
| 48  | 5     | 2046 | G    |
| 48  | 5     | 2068 | C    |
| 48  | 5     | 2083 | C    |
| 48  | 5     | 2084 | C    |
| 48  | 5     | 2088 | A    |
| 48  | 5     | 2089 | G    |
| 48  | 5     | 2093 | A    |
| 48  | 5     | 2107 | C    |
| 48  | 5     | 2110 | C    |
| 48  | 5     | 2116 | C    |
| 48  | 5     | 2119 | C    |
| 48  | 5     | 2122 | G    |
| 48  | 5     | 2123 | C    |
| 48  | 5     | 2125 | C    |
| 48  | 5     | 2246 | C    |
| 48  | 5     | 2251 | G    |
| 48  | 5     | 2253 | A    |
| 48  | 5     | 2256 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 2257 | C    |
| 48  | 5     | 2260 | C    |
| 48  | 5     | 2262 | G    |
| 48  | 5     | 2265 | G    |
| 48  | 5     | 2266 | C    |
| 48  | 5     | 2269 | C    |
| 48  | 5     | 2278 | G    |
| 48  | 5     | 2313 | A    |
| 48  | 5     | 2333 | G    |
| 48  | 5     | 2370 | A    |
| 48  | 5     | 2396 | A    |
| 48  | 5     | 2398 | U    |
| 48  | 5     | 2467 | U    |
| 48  | 5     | 2468 | U    |
| 48  | 5     | 2473 | A    |
| 48  | 5     | 2474 | G    |
| 48  | 5     | 2490 | U    |
| 48  | 5     | 2502 | G    |
| 48  | 5     | 2505 | C    |
| 48  | 5     | 2506 | G    |
| 48  | 5     | 2513 | A    |
| 48  | 5     | 2546 | G    |
| 48  | 5     | 2553 | A    |
| 48  | 5     | 2554 | U    |
| 48  | 5     | 2587 | A    |
| 48  | 5     | 2588 | C    |
| 48  | 5     | 2623 | A    |
| 48  | 5     | 2661 | U    |
| 48  | 5     | 2687 | U    |
| 48  | 5     | 2695 | A    |
| 48  | 5     | 2724 | G    |
| 48  | 5     | 2739 | C    |
| 48  | 5     | 2754 | G    |
| 48  | 5     | 2769 | U    |
| 48  | 5     | 2782 | U    |
| 48  | 5     | 2794 | C    |
| 48  | 5     | 2806 | A    |
| 48  | 5     | 2827 | G    |
| 48  | 5     | 2858 | A    |
| 48  | 5     | 3593 | C    |
| 48  | 5     | 3625 | G    |
| 48  | 5     | 3670 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 3673 | C    |
| 48  | 5     | 3697 | U    |
| 48  | 5     | 3702 | A    |
| 48  | 5     | 3709 | U    |
| 48  | 5     | 3710 | G    |
| 48  | 5     | 3713 | U    |
| 48  | 5     | 3715 | U    |
| 48  | 5     | 3717 | A    |
| 48  | 5     | 3752 | C    |
| 48  | 5     | 3784 | A    |
| 48  | 5     | 3876 | A    |
| 48  | 5     | 3878 | C    |
| 48  | 5     | 3888 | G    |
| 48  | 5     | 3904 | G    |
| 48  | 5     | 4069 | U    |
| 48  | 5     | 4075 | U    |
| 48  | 5     | 4084 | G    |
| 48  | 5     | 4086 | G    |
| 48  | 5     | 4115 | G    |
| 48  | 5     | 4119 | C    |
| 48  | 5     | 4121 | G    |
| 48  | 5     | 4124 | G    |
| 48  | 5     | 4144 | C    |
| 48  | 5     | 4170 | A    |
| 48  | 5     | 4232 | U    |
| 48  | 5     | 4254 | G    |
| 48  | 5     | 4331 | G    |
| 48  | 5     | 4349 | C    |
| 48  | 5     | 4378 | A    |
| 48  | 5     | 4395 | U    |
| 48  | 5     | 4404 | U    |
| 48  | 5     | 4448 | G    |
| 48  | 5     | 4449 | A    |
| 48  | 5     | 4463 | U    |
| 48  | 5     | 4475 | G    |
| 48  | 5     | 4510 | A    |
| 48  | 5     | 4512 | U    |
| 48  | 5     | 4527 | G    |
| 48  | 5     | 4528 | G    |
| 48  | 5     | 4548 | A    |
| 48  | 5     | 4583 | C    |
| 48  | 5     | 4656 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | 5     | 4694 | G    |
| 48  | 5     | 4699 | U    |
| 48  | 5     | 4718 | G    |
| 48  | 5     | 4719 | G    |
| 48  | 5     | 4730 | C    |
| 48  | 5     | 4872 | G    |
| 48  | 5     | 4885 | U    |
| 48  | 5     | 4888 | U    |
| 48  | 5     | 4889 | G    |
| 48  | 5     | 4895 | C    |
| 48  | 5     | 4900 | C    |
| 48  | 5     | 4926 | C    |
| 48  | 5     | 4935 | C    |
| 48  | 5     | 4948 | C    |
| 48  | 5     | 4951 | G    |
| 48  | 5     | 4965 | U    |
| 48  | 5     | 4975 | G    |
| 48  | 5     | 4990 | C    |
| 48  | 5     | 5022 | U    |
| 48  | 5     | 5026 | U    |
| 48  | 5     | 5027 | C    |
| 48  | 5     | 5047 | C    |
| 48  | 5     | 5059 | C    |
| 48  | 5     | 5060 | A    |
| 48  | 5     | 5061 | A    |
| 49  | 7     | 109  | U    |
| 50  | 8     | 2    | G    |
| 50  | 8     | 51   | U    |
| 50  | 8     | 94   | G    |
| 50  | 8     | 110  | U    |
| 50  | 8     | 111  | U    |
| 50  | 8     | 124  | U    |
| 51  | 9     | 1    | U    |
| 51  | 9     | 2    | A    |
| 51  | 9     | 3    | C    |
| 51  | 9     | 43   | U    |
| 51  | 9     | 44   | U    |
| 51  | 9     | 58   | C    |
| 51  | 9     | 62   | G    |
| 51  | 9     | 72   | C    |
| 51  | 9     | 92   | A    |
| 51  | 9     | 102  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 9     | 110 | U    |
| 51  | 9     | 113 | G    |
| 51  | 9     | 139 | C    |
| 51  | 9     | 140 | C    |
| 51  | 9     | 143 | U    |
| 51  | 9     | 146 | G    |
| 51  | 9     | 160 | U    |
| 51  | 9     | 164 | A    |
| 51  | 9     | 180 | G    |
| 51  | 9     | 183 | G    |
| 51  | 9     | 191 | A    |
| 51  | 9     | 215 | G    |
| 51  | 9     | 291 | G    |
| 51  | 9     | 292 | A    |
| 51  | 9     | 304 | C    |
| 51  | 9     | 305 | U    |
| 51  | 9     | 312 | G    |
| 51  | 9     | 321 | C    |
| 51  | 9     | 322 | C    |
| 51  | 9     | 327 | G    |
| 51  | 9     | 369 | C    |
| 51  | 9     | 400 | C    |
| 51  | 9     | 407 | G    |
| 51  | 9     | 434 | G    |
| 51  | 9     | 447 | A    |
| 51  | 9     | 448 | A    |
| 51  | 9     | 464 | A    |
| 51  | 9     | 465 | A    |
| 51  | 9     | 473 | A    |
| 51  | 9     | 488 | U    |
| 51  | 9     | 500 | A    |
| 51  | 9     | 532 | C    |
| 51  | 9     | 550 | C    |
| 51  | 9     | 559 | G    |
| 51  | 9     | 589 | G    |
| 51  | 9     | 594 | A    |
| 51  | 9     | 606 | G    |
| 51  | 9     | 620 | G    |
| 51  | 9     | 627 | U    |
| 51  | 9     | 642 | U    |
| 51  | 9     | 656 | G    |
| 51  | 9     | 670 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 688  | U    |
| 51  | 9     | 746  | C    |
| 51  | 9     | 747  | U    |
| 51  | 9     | 752  | G    |
| 51  | 9     | 797  | C    |
| 51  | 9     | 798  | G    |
| 51  | 9     | 833  | C    |
| 51  | 9     | 844  | U    |
| 51  | 9     | 869  | A    |
| 51  | 9     | 870  | A    |
| 51  | 9     | 887  | U    |
| 51  | 9     | 912  | C    |
| 51  | 9     | 913  | A    |
| 51  | 9     | 970  | G    |
| 51  | 9     | 1016 | U    |
| 51  | 9     | 1087 | A    |
| 51  | 9     | 1109 | C    |
| 51  | 9     | 1113 | A    |
| 51  | 9     | 1115 | U    |
| 51  | 9     | 1137 | U    |
| 51  | 9     | 1138 | C    |
| 51  | 9     | 1165 | G    |
| 51  | 9     | 1212 | G    |
| 51  | 9     | 1234 | C    |
| 51  | 9     | 1247 | C    |
| 51  | 9     | 1253 | A    |
| 51  | 9     | 1265 | A    |
| 51  | 9     | 1275 | G    |
| 51  | 9     | 1283 | C    |
| 51  | 9     | 1294 | G    |
| 51  | 9     | 1298 | G    |
| 51  | 9     | 1302 | G    |
| 51  | 9     | 1308 | U    |
| 51  | 9     | 1309 | C    |
| 51  | 9     | 1312 | G    |
| 51  | 9     | 1313 | A    |
| 51  | 9     | 1330 | G    |
| 51  | 9     | 1342 | U    |
| 51  | 9     | 1394 | G    |
| 51  | 9     | 1395 | C    |
| 51  | 9     | 1396 | A    |
| 51  | 9     | 1407 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | 9     | 1418 | C    |
| 51  | 9     | 1419 | C    |
| 51  | 9     | 1432 | U    |
| 51  | 9     | 1438 | A    |
| 51  | 9     | 1448 | A    |
| 51  | 9     | 1454 | A    |
| 51  | 9     | 1455 | A    |
| 51  | 9     | 1475 | G    |
| 51  | 9     | 1477 | U    |
| 51  | 9     | 1489 | A    |
| 51  | 9     | 1508 | A    |
| 51  | 9     | 1534 | C    |
| 51  | 9     | 1555 | U    |
| 51  | 9     | 1580 | A    |
| 51  | 9     | 1601 | A    |
| 51  | 9     | 1621 | U    |
| 51  | 9     | 1623 | A    |
| 51  | 9     | 1632 | G    |
| 51  | 9     | 1636 | G    |
| 51  | 9     | 1637 | A    |
| 51  | 9     | 1638 | G    |
| 51  | 9     | 1646 | C    |
| 51  | 9     | 1647 | A    |
| 51  | 9     | 1664 | A    |
| 51  | 9     | 1665 | G    |
| 51  | 9     | 1679 | A    |
| 51  | 9     | 1680 | G    |
| 51  | 9     | 1721 | U    |
| 51  | 9     | 1724 | A    |
| 51  | 9     | 1728 | U    |
| 51  | 9     | 1824 | A    |
| 51  | 9     | 1826 | G    |
| 51  | 9     | 1830 | U    |
| 51  | 9     | 1835 | A    |
| 51  | 9     | 1837 | 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 207 ligands modelled in this entry, 203 are monoatomic - leaving 4 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$ |
| 90  | SF4  | jj    | 600 | 87   | 0,12,12      | 0.00 | -           | 0,24,24     | 0.00 | -           |
| 90  | SF4  | jj    | 601 | 87   | 0,12,12      | 0.00 | -           | 0,24,24     | 0.00 | -           |
| 91  | ADP  | jj    | 602 | -    | 24,29,29     | 1.07 | 1 (4%)      | 23,45,45    | 1.92 | 1 (4%)      |
| 91  | ADP  | jj    | 603 | -    | 24,29,29     | 1.08 | 2 (8%)      | 23,45,45    | 1.91 | 1 (4%)      |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 90  | SF4  | jj    | 600 | 87   | -       | 0/0/48/48  | 0/6/5/5 |
| 90  | SF4  | jj    | 601 | 87   | -       | 0/0/48/48  | 0/6/5/5 |
| 91  | ADP  | jj    | 602 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 91  | ADP  | jj    | 603 | -    | -       | 0/12/32/32 | 0/3/3/3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 91  | jj    | 603 | ADP  | C2-N3 | 2.06 | 1.35        | 1.32     |
| 91  | jj    | 602 | ADP  | C5-C4 | 3.28 | 1.47        | 1.40     |
| 91  | jj    | 603 | ADP  | C5-C4 | 3.34 | 1.48        | 1.40     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|----------|-------|------------------------|---------------------|
| 91  | jj    | 602 | ADP  | N3-C2-N1 | -7.73 | 122.80                 | 128.87              |
| 91  | jj    | 603 | ADP  | N3-C2-N1 | -7.72 | 122.81                 | 128.87              |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.