



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:45 PM UTC

PDB ID : 8IFD / pdb\_00008ifd  
EMDB ID : EMD-35413  
Title : Dibekacin-added human 80S ribosome  
Authors : Tomono, J.; Asano, K.; Chiashi, T.; Tanaka, Y.; Yokoyama, T.  
Deposited on : 2023-02-17  
Resolution : 2.59 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

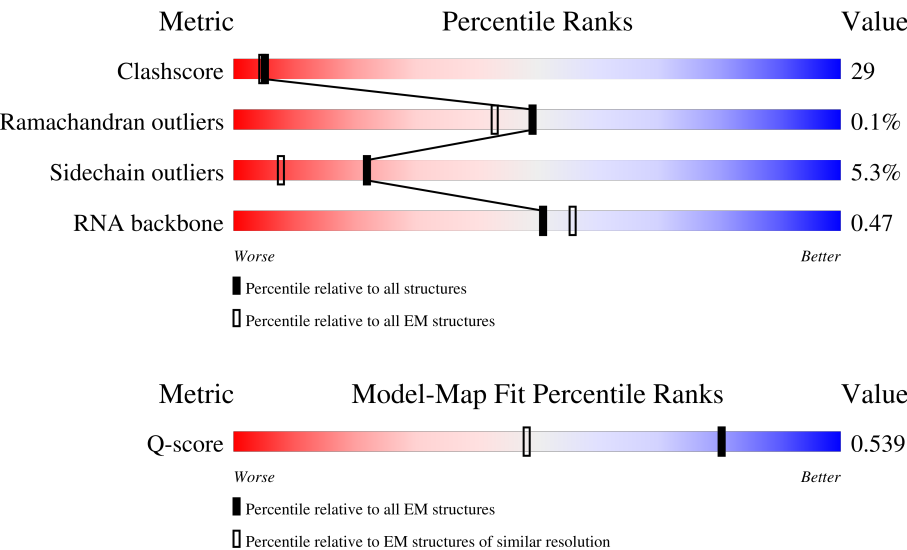
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.59 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 7741 ( 2.09 - 3.09 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1A    | 5070   |                  |
| 2   | 1B    | 121    |                  |
| 3   | 1C    | 157    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 1D    | 257    |                  |
| 5   | 1E    | 403    |                  |
| 6   | 1F    | 427    |                  |
| 7   | 1G    | 297    |                  |
| 8   | 1H    | 288    |                  |
| 9   | 2A    | 248    |                  |
| 10  | 2B    | 266    |                  |
| 11  | 2C    | 192    |                  |
| 12  | 2D    | 214    |                  |
| 13  | 2E    | 178    |                  |
| 14  | 2F    | 211    |                  |
| 15  | 2G    | 215    |                  |
| 16  | 2H    | 204    |                  |
| 17  | 2I    | 203    |                  |
| 18  | 2J    | 184    |                  |
| 19  | 2K    | 188    |                  |
| 20  | 2L    | 196    |                  |
| 21  | 2M    | 176    |                  |
| 22  | 2N    | 160    |                  |
| 23  | 2O    | 128    |                  |
| 24  | 2P    | 140    |                  |
| 25  | 2Q    | 157    |                  |
| 26  | 2R    | 156    |                  |
| 27  | 2S    | 145    |                  |
| 28  | 2T    | 136    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | 2U    | 148    |                  |
| 30  | 2V    | 159    |                  |
| 31  | 2W    | 115    |                  |
| 32  | 2X    | 125    |                  |
| 33  | 2Y    | 135    |                  |
| 34  | 2Z    | 110    |                  |
| 35  | 2a    | 117    |                  |
| 36  | 2b    | 123    |                  |
| 37  | 2c    | 105    |                  |
| 38  | 2d    | 97     |                  |
| 39  | 2e    | 70     |                  |
| 40  | 2f    | 51     |                  |
| 41  | 2g    | 128    |                  |
| 42  | 2h    | 25     |                  |
| 43  | 2i    | 106    |                  |
| 44  | 2j    | 92     |                  |
| 45  | 2k    | 137    |                  |
| 46  | 2l    | 217    |                  |
| 47  | 2m    | 1869   |                  |
| 48  | 2n    | 295    |                  |
| 49  | 2o    | 264    |                  |
| 50  | 2p    | 243    |                  |
| 51  | 2q    | 263    |                  |
| 52  | 2r    | 204    |                  |
| 53  | 2s    | 194    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | 2t    | 208    |                  |
| 55  | 2u    | 165    |                  |
| 56  | 2v    | 158    |                  |
| 57  | 2w    | 145    |                  |
| 58  | 2x    | 146    |                  |
| 59  | 2y    | 135    |                  |
| 60  | 2z    | 152    |                  |
| 61  | 20    | 145    |                  |
| 62  | 21    | 119    |                  |
| 63  | 3A    | 83     |                  |
| 64  | 3B    | 143    |                  |
| 65  | 3C    | 115    |                  |
| 66  | 3D    | 69     |                  |
| 67  | 3E    | 56     |                  |
| 68  | 3F    | 317    |                  |
| 69  | 3G    | 293    |                  |
| 70  | 3H    | 249    |                  |
| 71  | 3I    | 194    |                  |
| 72  | 3J    | 132    |                  |
| 73  | 3K    | 151    |                  |
| 74  | 3L    | 151    |                  |
| 75  | 3M    | 130    |                  |
| 76  | 3N    | 133    |                  |
| 77  | 3O    | 125    |                  |
| 78  | 3P    | 84     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                                            |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------------------------|
| 79  | 3Q    | 59     | <div><div><div></div><div></div><div></div></div><div>54%</div><div>53%</div><div>44%</div><div>••</div></div>              |
| 80  | 3R    | 156    | <div><div><div></div><div></div><div></div></div><div>43%</div><div>22%</div><div>19%</div><div>•</div><div>57%</div></div> |

## 2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 218821 atoms, of which 888 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 RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | 1A    | 3717     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 79674 | 35479 | 14585 | 25894 | 3716 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| 1A    | 2113    | C        | G      | conflict | GB 86475748 |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2   | 1B    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | 1C    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3310  | 1477 | 585 | 1093 | 155 |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | 1D    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 1E    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3238  | 2060 | 608 | 556 | 14 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 1F    | 368      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2927  | 1840 | 583 | 489 | 15 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | 1G    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2382  | 1507 | 434 | 427 | 14 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | 1H    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1904  | 1222 | 361 | 317 | 4 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | 2A    | 225      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1878  | 1207 | 361 | 301 | 9 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | 2B    | 241      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1935  | 1233 | 374 | 324 | 4 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | 2C    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | 2D    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1711  | 1082 | 329 | 285 | 15 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L11.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | 2E    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 888 | 263 | 253 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | 2F    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | 2G    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 730 | 218 | 183 | 7 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 2H    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | 2I    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | 2J    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | 2K    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | 2L    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 971 | 336 | 250 | 9 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | 2M    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 2N    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | 2O    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 529 | 144 | 150 | 2 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | 2P    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | 2Q    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 634 | 207 | 170 | 4 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | 2R    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 630 | 185 | 169 | 1 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | 2S    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | 2T    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | 2U    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | 2V    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 882   | 549 | 192 | 137 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | 2W    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | 2X    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | 2Y    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | 2Z    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | 2a    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | 2b    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | 2c    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | 2d    | 86       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 713   | 439 | 158 | 111 | 5 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 39  | 2e    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | 2f    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | 2g    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 430   | 267 | 90 | 67 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | 2h    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | 2i    | 105      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 870   | 547 | 178 | 139 | 6 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | 2j    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | 2k    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | 2l    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1740  | 1113 | 312 | 306 | 9 |         |       |

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 47  | 2m    | 1742     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36900 | 16458 | 6595 | 12106 | 1741 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference |
|-------|---------|----------|--------|----------|-----------|
| 2m    | 582     | C        | U      | conflict | GB 36162  |
| 2m    | 583     | C        | A      | conflict | GB 36162  |
| 2m    | 584     | G        | A      | conflict | GB 36162  |
| 2m    | 798     | A        | G      | conflict | GB 36162  |
| 2m    | 1095    | U        | C      | conflict | GB 36162  |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | 2n    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1106 | 305 | 322 | 8 |         |       |

- Molecule 49 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | 2o    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | 2p    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | 2q    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | 2r    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | 2s    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1497  | 956 | 274 | 266 | 1 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | 2t    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | 2u    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | 2v    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 793 | 234 | 214 | 6 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | 2w    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 663 | 198 | 177 | 7 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | 2x    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 715 | 212 | 194 | 3 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | 2y    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 685 | 202 | 198 | 5 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | 2z    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 751 | 242 | 203 | 2 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | 20    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 697 | 214 | 198 | 3 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | 21    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 511 | 155 | 147 | 4 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | 3A    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | 3B    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | 3C    | 102      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 829   | 517 | 174 | 133 | 5 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 66  | 3D    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 67  | 3E    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 68 is a protein called Receptor of activated protein C kinase 1.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 68  | 3F    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 69  | 3G    | 222      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1733  | 1120 | 301 | 302 | 10 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 70  | 3H    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | 3I    | 185      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1533  | 974 | 309 | 248 | 2 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | 3J    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 590 | 165 | 179 | 8 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 3J    | 52      | GLN      | LEU    | conflict | UNP P25398 |
| 3J    | 69      | LEU      | CYS    | conflict | UNP P25398 |
| 3J    | 99      | ASN      | LYS    | conflict | UNP P25398 |

- Molecule 73 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | 3K    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | 3L    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 642 | 204 | 197 | 6 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | 3M    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | 3N    | 131      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1073  | 678 | 212 | 178 | 5 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | 3O    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | 3P    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

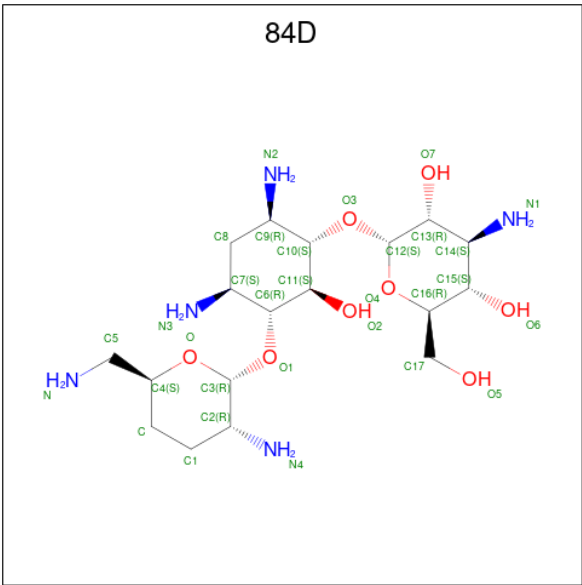
- Molecule 79 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 79  | 3Q    | 58       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 459   | 284 | 100 | 74 | 1 |         |       |

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 80  | 3R    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 548   | 346 | 102 | 93 | 7 |         |       |

- Molecule 81 is Dibekacin (CCD ID: 84D) (formula:  $C_{18}H_{37}N_5O_8$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 1A    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 2m    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 2m    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |
| 81  | 2m    | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 68    | 18 | 37 | 5 | 8 |         |

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 82  | 1A    | 270      | Total | Mg  | 0       |
|     |       |          | 270   | 270 |         |
| 82  | 1B    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 82  | 1C    | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 82  | 1D    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 82  | 2H    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 82  | 2J    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 82  | 2K    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 82  | 2M    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 82  | 2P    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

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| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 82  | 2V    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 2Y    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 2Z    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 2a    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 2d    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 2m    | 105      | Total<br>105 | Mg<br>105 | 0       |
| 82  | 2o    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 3H    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 3K    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 82  | 3L    | 1        | Total<br>1   | Mg<br>1   | 0       |

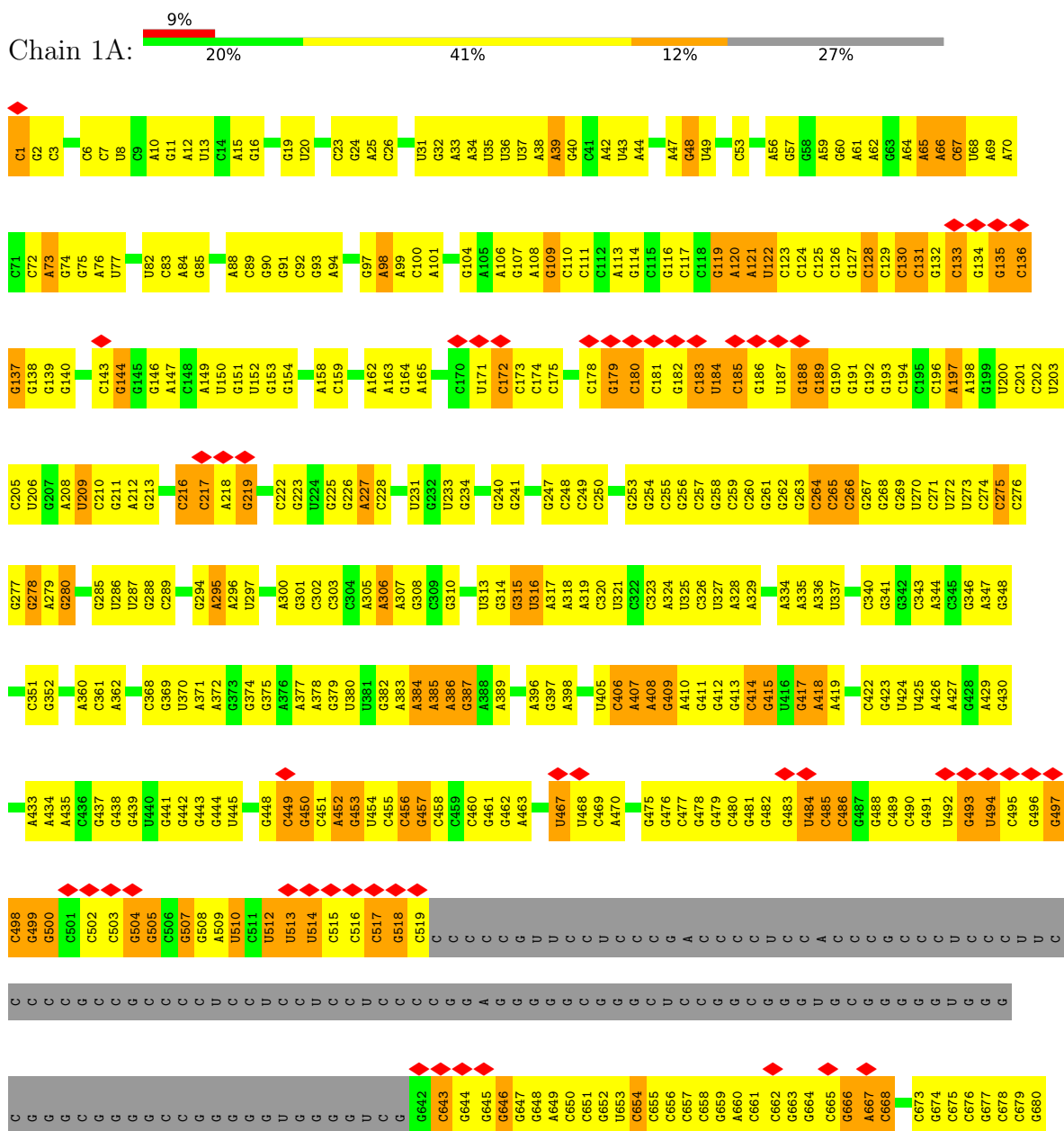
- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

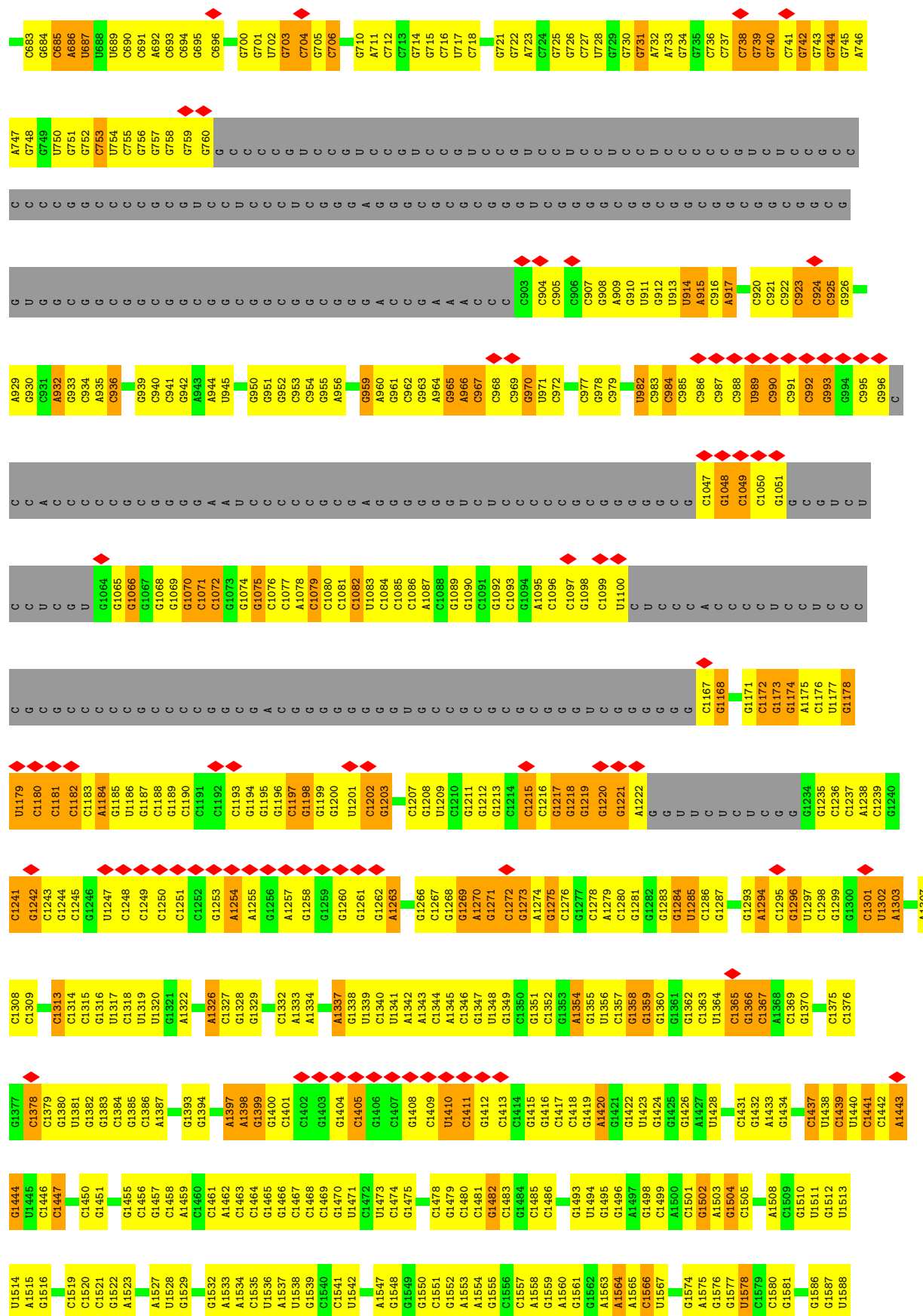
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 83  | 2d    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 83  | 2g    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 83  | 2j    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 83  | 3C    | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

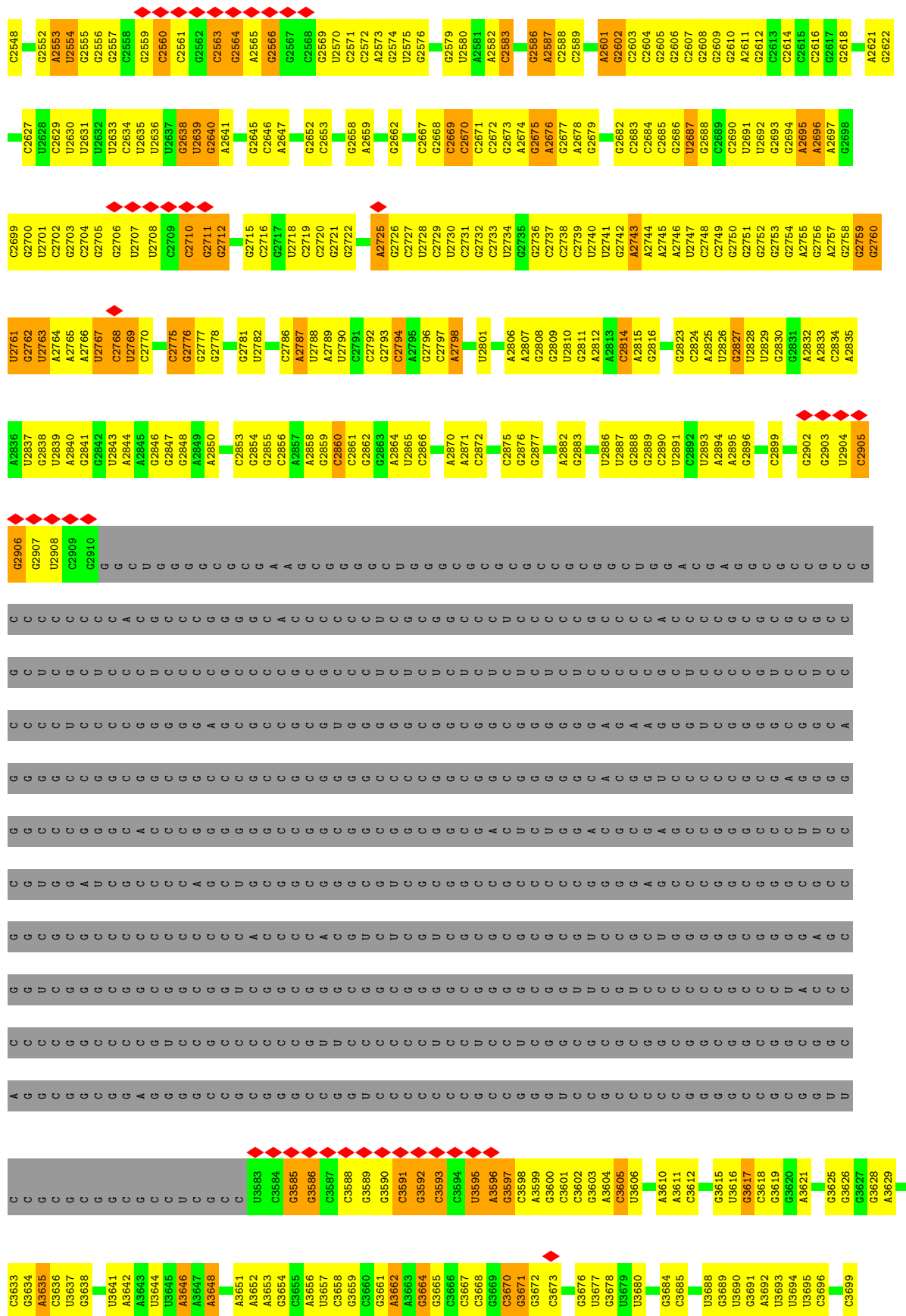
#### • Molecule 1: 28S ribosomal RNA



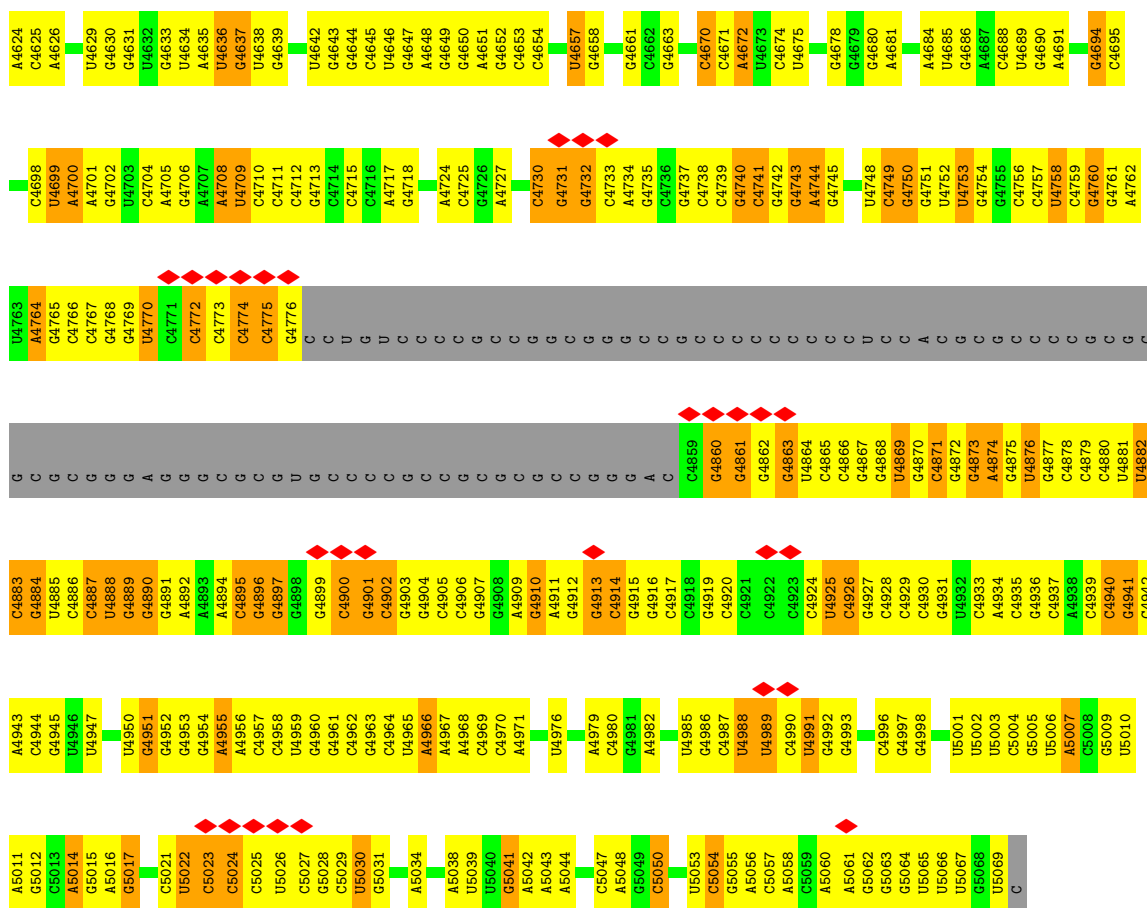




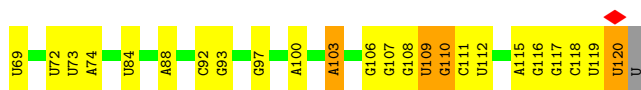




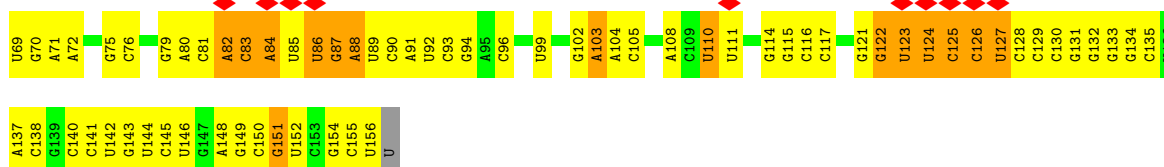
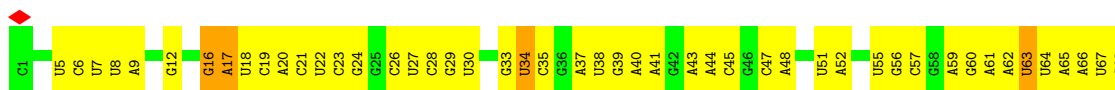
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C4560 | C4485 | G4418 | C4349 | A4281 | U4218 | G4151 | G4090 | C     | G3969 | A3908 | G3839 | C3771 | C3700 |
| A4487 | C4486 | U4419 | C4350 | A4282 | A4219 | G4152 | G4091 | C     | G3970 | C3909 | U3840 | U3772 | G3701 |
| U4492 | A4487 | C4420 | U4351 | C4283 | A4220 | C4153 | G4092 | U     | G3971 | C3910 | A3845 | A3774 | A3702 |
| U4495 | U4492 | C4421 | U4352 | C4284 | A4221 | C4154 | G4093 | G     | A3972 | C3911 | C3847 | C3775 | C3706 |
| G4495 | U4495 | U4423 | U4353 | U4285 | G4222 | C4155 | G4094 | C     | G3973 | U3912 | U3848 | G3776 | U3707 |
| A4424 | G4495 | A4424 | G4356 | C4288 | G4226 | A4157 | G4095 | G4034 | G3974 | U3914 | A3849 | U3777 | C3708 |
| G4425 | U4499 | G4425 | U4357 | U4289 | U4227 | C4158 | G4096 | G4035 | C3975 | U3915 | C3850 | G3710 | U3709 |
| A4428 | U4500 | G4427 | U4358 | U4290 | G4228 | C4159 | G4097 | G4036 | C3976 | A3917 | C3781 | A3711 | A3712 |
| C4429 | U4501 | A4428 | U4359 | G4291 | U4229 | U4162 | A4098 | C4037 | C3977 | G3918 | C3782 | C3782 | U3713 |
| G4430 | C4429 | C4429 | U4360 | U4296 | C4230 | C4164 | G4099 | C4038 | C     | C3919 | A3855 | U3714 | G3715 |
| U4437 | U4502 | G4429 | G4297 | G4297 | C4232 | G4165 | C4100 | G4039 | C     | U3920 | C3857 | A3785 | C3716 |
| U4438 | U4503 | G4430 | U4371 | A4305 | A4233 | G4166 | C4101 | C4040 | C     | U3921 | C3858 | U3786 | A3717 |
| U4439 | C4505 | U4438 | U4372 | G4306 | A4234 | C4167 | C4102 | C4041 | C     | A3922 | C3860 | A3718 | G3719 |
| A4441 | U4506 | G4433 | A4375 | A4307 | G4236 | G4168 | C4103 | G4042 | C     | C3924 | A3861 | A3719 | G3720 |
| U4442 | A4507 | C4434 | A4376 | U4311 | C4237 | C4169 | G4104 | G4043 | C     | U3925 | A3862 | A3721 | U3721 |
| C4443 | U4436 | U4436 | G4377 | U4312 | G4238 | A4170 | A4104 | G4044 | C     | A3928 | A3865 | C3794 | C3722 |
| G4444 | U4437 | U4437 | A4378 | A4313 | A4243 | G4171 | A4105 | U4044 | C     | U3930 | C3866 | A3795 | A3723 |
| U4445 | U4438 | C4444 | A4379 | A4314 | G4245 | G4172 | C4110 | U4045 | C     | U3931 | C3868 | U3796 | A3724 |
| U4446 | U4439 | U4446 | A4380 | A4315 | G4246 | G4173 | U4111 | A4050 | C     | U3932 | C3869 | C3797 | G3725 |
| U4447 | U4440 | G4447 | A4381 | A4316 | G4247 | G4174 | U4112 | C4051 | C     | C3933 | C3870 | U3798 | A3726 |
| U4448 | U4441 | G4448 | A4382 | G4317 | A4248 | U4175 | C4113 | C4052 | C     | C3934 | A3871 | A3727 | A3728 |
| A4449 | U4442 | A4449 | A4383 | C4318 | G4250 | G4176 | U4114 | C4053 | C     | A3935 | A3872 | A3800 |       |
| U4450 | U4453 | U4450 | U4384 | C4319 | A4251 | G4177 | C4115 | C4054 | C     | C3936 | C3873 | U3801 | A3732 |
| U4451 | U4454 | U4451 | A4385 | G4320 | A4252 | G4178 | G4116 | U4055 | C     | C3937 | C3874 | U3802 | A3733 |
| U4452 | U4455 | U4452 | A4386 | U4321 | G4253 | G4179 | U4117 | U4056 | C     | C3938 | A3877 | A3803 | A3734 |
| C4453 | U4456 | C4453 | A4387 | G4322 | A4254 | G4180 | G4118 | A4057 | C     | U3939 | C3878 | A3807 | G3735 |
| G4454 | U4457 | G4454 | A4388 | A4323 | A4255 | U4189 | C4119 | C4057 | C     | G3940 | C3879 | C3808 | A3736 |
| U4457 | U4458 | U4457 | C4389 | A4324 | A4256 | U4190 | U4120 | U4058 | C     | A3942 | C3880 | A3737 | G3738 |
| C4458 | C4458 | C4458 | A4390 | A4325 | A4257 | G4191 | G4121 | C4059 | C     | G3944 | C3881 | C3810 |       |
| U4459 | U4459 | U4459 | A4391 | A4326 | C4258 | A4192 | C4122 | U4060 | C     | A3945 | C3882 | C3811 | A3746 |
| U4460 | U4460 | U4460 | G4392 | G4327 | U4259 | C4193 | G4123 | U4061 | C     | G3946 | U3883 | C3812 | A3747 |
| C4461 | C4461 | C4461 | A4393 | G4328 | G4261 | U4194 | G4124 | G4062 | C     | C3947 | U3884 | U3814 | A3748 |
| U4463 | C4462 | U4463 | U4394 | G4329 | C4262 | G4197 | C4125 | A4063 | C     | C3948 | G3885 | G3815 |       |
| U4464 | U4464 | U4464 | A4395 | A4330 | G4263 | U4198 | C4126 | U4064 | C     | A3949 | C3888 | A3816 | G3751 |
| U4465 | U4465 | U4465 | A4396 | C4331 | G4264 | C4199 | A4127 | U4065 | C     | U3950 | C3889 | A3817 | G3752 |
| C4466 | U4466 | U4466 | C4397 | C4332 | U4265 | G4200 | G4128 | C4066 | C     | G3951 | A3890 | U3818 | G3753 |
| A4467 | A4467 | A4467 | U4398 | C4333 | G4266 | U4201 | C4129 | U4067 | C     | C3952 | A3891 | G3819 | G3754 |
| U4468 | U4468 | U4468 | G4401 | U4334 | G4267 | C4202 | G4130 | U4068 | C     | G3953 | U3892 | G3820 | G3755 |
| G4472 | G4472 | G4472 | C4402 | C4337 | A4268 | C4204 | C4132 | U4069 | C     | A3954 | C3895 | A3821 | A3756 |
| A4473 | A4473 | A4473 | U4403 | A4338 | G4269 | G4205 | C4133 | U4070 | C     | G3955 | C3896 | G3822 | G3757 |
| U4474 | U4474 | U4474 | U4404 | A4339 | C4270 | C4206 | G4134 | U4071 | C     | C3956 | C3897 | A3824 | U3758 |
| C4475 | C4475 | C4475 | G4407 | C4340 | G4271 | U4208 | G4135 | U4072 | C     | U3957 | G3898 | A3825 | A3759 |
| C4476 | C4476 | C4476 | U4408 | C4341 | G4272 | U4209 | G4136 | C4073 | C     | G3829 | G3899 | G3825 | A3760 |
| U4480 | U4480 | U4480 | C4412 | C4342 | A4274 | U4210 | C4137 | U4074 | C     | U3830 | C3900 | U3762 | C3761 |
| U4481 | U4481 | U4481 | U4413 | U4343 | G4275 | C4211 | C4138 | A4075 | C     | U3832 | C3901 | U3763 | U3764 |
| U4482 | U4482 | U4482 | A4414 | U4344 | G4276 | A4212 | G4139 | U4076 | C     | A3960 | A3902 | C3833 | C3833 |
| U4483 | U4483 | U4483 | A4415 | C4345 | G4277 | A4214 | C4140 | U4077 | C     | G3961 | C3903 | C3834 | C3765 |
| U4484 | U4484 | U4484 | G4416 | U4346 | C4278 | C4215 | C4141 | G4078 | C     | A3962 | A3904 | C3835 | A3766 |
| U4485 | U4485 | U4485 | C4417 | A4348 | A4280 | G4216 | G4142 | U4079 | C     | A3963 | A3905 | A3836 | C3767 |
| U4486 | U4486 | U4486 | U4417 | U4349 |       | C4217 | C4143 | C4080 | C     | U3964 | A3906 | C3837 | U3768 |
| U4487 | U4487 | U4487 | U4418 | U4350 |       | G4218 | C4144 | G4081 | C     | A3965 | C3907 | U3838 | C3769 |
| U4488 | U4488 | U4488 | U4419 | U4351 |       | G4219 | C4145 | G4082 | C     | G3967 |       |       | U3770 |
| U4489 | U4489 | U4489 | U4420 | U4352 |       | G4220 | G4146 | U4083 | C     | U3968 |       |       |       |
| U4490 | U4490 | U4490 | U4421 | U4353 |       | G4221 | G4147 | A4084 | C     |       |       |       |       |
| U4491 | U4491 | U4491 | U4422 | U4354 |       | G4222 | G4148 | A4085 | C     |       |       |       |       |
| U4492 | U4492 | U4492 | U4423 | U4355 |       | G4223 | G4149 | A4086 | C     |       |       |       |       |
| U4493 | U4493 | U4493 | U4424 | U4356 |       | G4224 | G4150 | A4087 | C     |       |       |       |       |
| U4494 | U4494 | U4494 | U4425 | U4357 |       | G4225 | G4151 | A4088 | C     |       |       |       |       |
| U4495 | U4495 | U4495 | U4426 | U4358 |       | G4226 | G4152 | A4089 | C     |       |       |       |       |
| U4496 | U4496 | U4496 | U4427 | U4359 |       | G4227 | G4153 | A4090 | C     |       |       |       |       |
| U4497 | U4497 | U4497 | U4428 | U4360 |       | G4228 | G4154 | A4091 | C     |       |       |       |       |
| U4498 | U4498 | U4498 | U4429 | U4361 |       | G4229 | G4155 | A4092 | C     |       |       |       |       |
| U4499 | U4499 | U4499 | U4430 | U4362 |       | G4230 | G4156 | A4093 | C     |       |       |       |       |
| U4500 | U4500 | U4500 | U4431 | U4363 |       | G4231 | G4157 | A4094 | C     |       |       |       |       |
| U4501 | U4501 | U4501 | U4432 | U4364 |       | G4232 | G4158 | A4095 | C     |       |       |       |       |
| U4502 | U4502 | U4502 | U4433 | U4365 |       | G4233 | G4159 | A4096 | C     |       |       |       |       |
| U4503 | U4503 | U4503 | U4434 | U4366 |       | G4234 | G4160 | A4097 | C     |       |       |       |       |
| U4504 | U4504 | U4504 | U4435 | U4367 |       | G4235 | G4161 | A4098 | C     |       |       |       |       |
| U4505 | U4505 | U4505 | U4436 | U4368 |       | G4236 | G4162 | A4099 | C     |       |       |       |       |
| U4506 | U4506 | U4506 | U4437 | U4369 |       | G4237 | G4163 | A4100 | C     |       |       |       |       |
| U4507 | U4507 | U4507 | U4438 | U4370 |       | G4238 | G4164 | C4101 | C     |       |       |       |       |
| U4508 | U4508 | U4508 | U4439 | U4371 |       | G4239 | G4165 | C4102 | C     |       |       |       |       |
| U4509 | U4509 | U4509 | U4440 | U4372 |       | G4240 | G4166 | C4103 | C     |       |       |       |       |
| U4510 | U4510 | U4510 | U4441 | U4373 |       | G4241 | G4167 | C4104 | C     |       |       |       |       |
| U4511 | U4511 | U4511 | U4442 | U4374 |       | G4242 | G4168 | C4105 | C     |       |       |       |       |
| U4512 | U4512 | U4512 | U4443 | U4375 |       | G4243 | G4169 | C4106 | C     |       |       |       |       |
| U4513 | U4513 | U4513 | U4444 | U4376 |       | G4244 | G4170 | C4107 | C     |       |       |       |       |
| U4514 | U4514 | U4514 | U4445 | U4377 |       | G4245 | G4171 | G4108 | C     |       |       |       |       |
| U4515 | U4515 | U4515 | U4446 | U4378 |       | G4246 | G4172 | G4109 | C     |       |       |       |       |
| U4516 | U4516 | U4516 | U4447 | U4379 |       | G4247 | G4173 | G4110 | C     |       |       |       |       |
| U4517 | U4517 | U4517 | U4448 | U4380 |       | G4248 | G4174 | G4111 | C     |       |       |       |       |
| U4518 | U4518 | U4518 | U4449 | U4381 |       | G4249 | G4175 | G4112 | C     |       |       |       |       |
| U4519 | U4519 | U4519 | U4450 | U4382 |       | G4250 | G4176 | G4113 | C     |       |       |       |       |
| U4520 | U4520 | U4520 | U4451 | U4383 |       | G4251 | G4177 | G4114 | C     |       |       |       |       |
| U4521 | U4521 | U4521 | U4452 | U4384 |       | G4252 | G4178 | G4115 | C     |       |       |       |       |
| U4522 | U4522 | U4522 | U4453 | U4385 |       | G4253 | G4179 | G4116 | C     |       |       |       |       |
| U4523 | U4523 | U4523 | U4454 | U4386 |       | G4254 | G4180 | G4117 | C     |       |       |       |       |
| U4524 | U4524 | U4524 | U4455 | U4387 |       | G4255 | G4181 | G4118 | C     |       |       |       |       |
| U4525 | U4525 | U4525 | U4456 | U4388 |       | G4256 | G4182 | G4119 | C     |       |       |       |       |
| U4526 | U4526 | U4526 | U4457 | U4389 |       | G4257 | G4183 | G4120 | C     |       |       |       |       |
| U4527 | U4527 | U4527 | U4458 | U4390 |       | G4258 | G4184 | G4121 | C     |       |       |       |       |
| U4528 | U4528 | U4528 | U4459 | U4391 |       | G4259 | G4185 | G4122 | C     |       |       |       |       |
| U4529 | U4529 | U4529 | U4460 | U4392 |       | G4260 | G4186 | G4123 | C     |       |       |       |       |
| U4530 | U4530 | U4530 | U4461 | U4393 |       | G4261 | G4187 | G4124 | C     |       |       |       |       |
| U4531 | U4531 | U4531 | U4462 | U4394 |       | G4262 | G4188 | G4125 | C     |       |       |       |       |
| U4532 | U4532 | U4532 | U4463 | U4395 |       | G4263 | G4189 | G4126 | C     |       |       |       |       |
| U4533 | U4533 | U4533 | U4464 | U4396 |       | G4264 | G4190 | G4127 | C     |       |       |       |       |
| U4534 | U4534 | U4534 | U4465 | U4397 |       | G4265 | G4191 | G4128 | C     |       |       |       |       |
| U4535 | U4535 | U4535 | U4466 | U4398 |       | G4266 | G4192 | G4129 | C     |       |       |       |       |
| U4536 | U4536 | U4536 | U4467 | U4399 |       | G4267 | G4193 | G4130 | C     |       |       |       |       |
| U4537 | U4537 | U4537 | U4468 | U4400 |       | G4268 | G4194 | G4131 | C     |       |       |       |       |
| U4538 | U4538 | U4538 | U4469 | U4401 |       | G4269 | G4195 | G4132 | C     |       |       |       |       |
| U4539 | U4539 | U4539 | U4470 | U4402 |       | G4270 | G4196 | G4133 | C     |       |       |       |       |
| U4540 | U4540 | U4540 | U4471 | U4403 |       | G4271 | G4197 | G4134 | C     |       |       |       |       |



### • Molecule 2: 5S ribosomal RNA

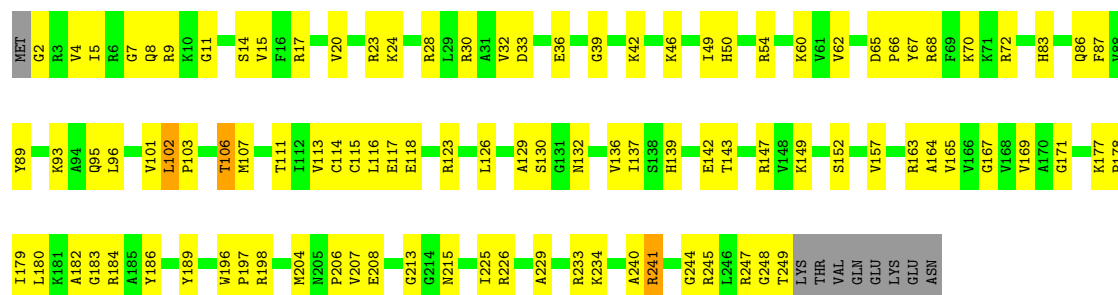


### • Molecule 3: 5.8S ribosomal RNA



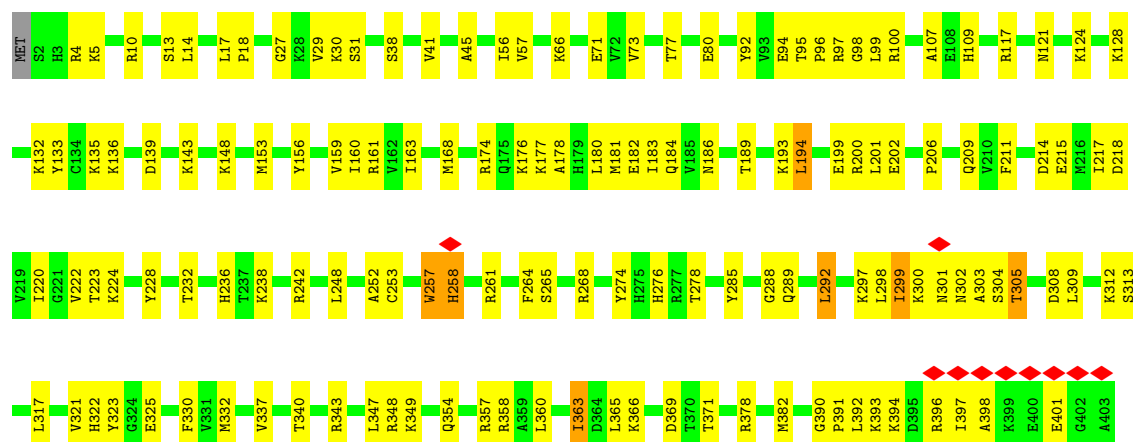
• Molecule 4: 60S ribosomal protein L8

Chain 1D:  57% 38%



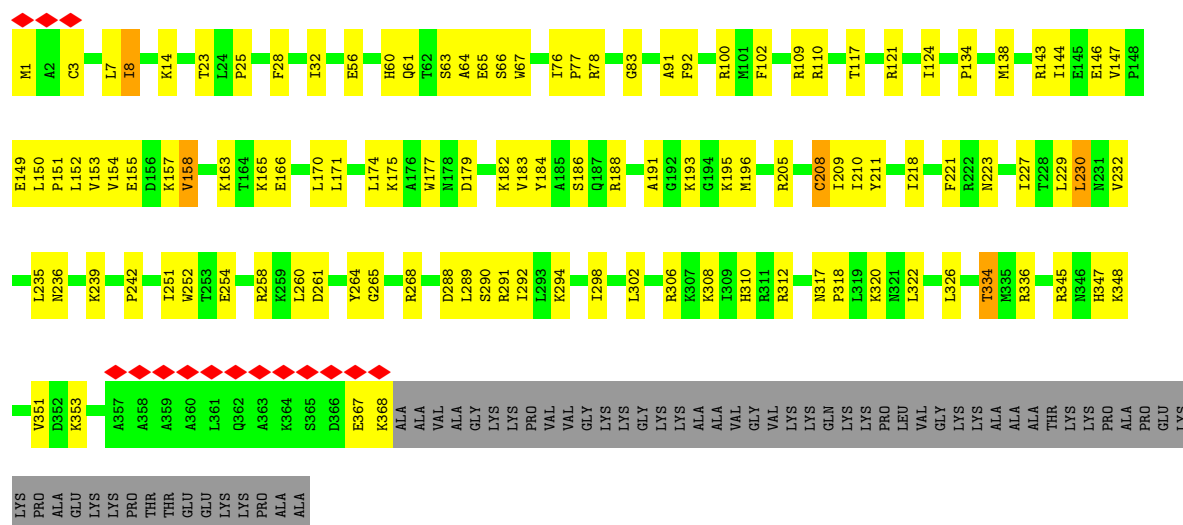
• Molecule 5: 60S ribosomal protein L3

Chain 1E:  64% 34%



• Molecule 6: 60S ribosomal protein L4

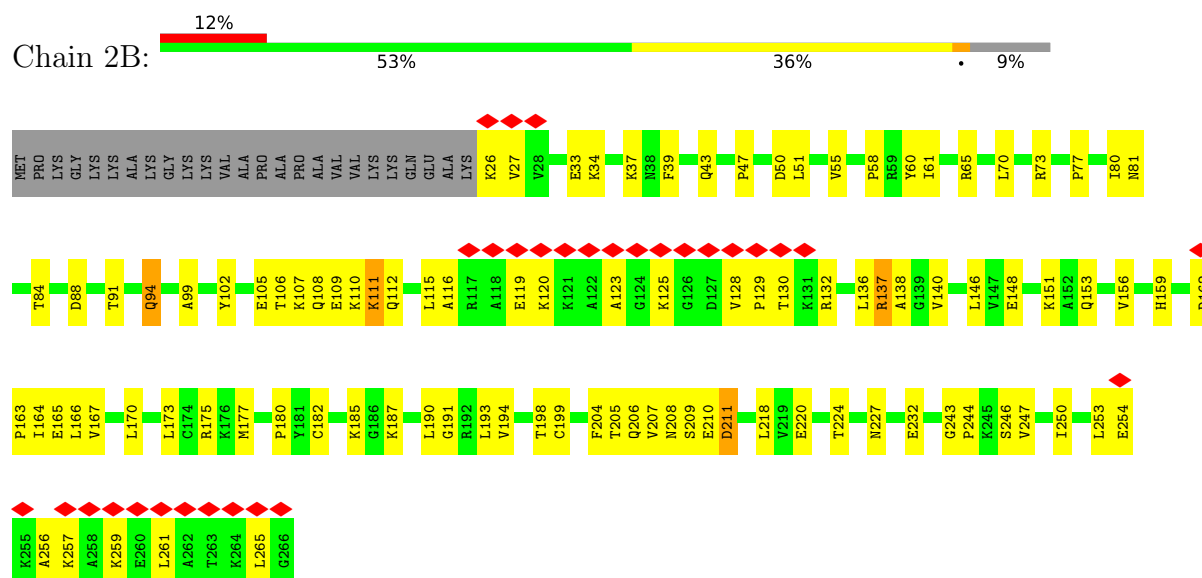
Chain 1F:  59% 26% 14%



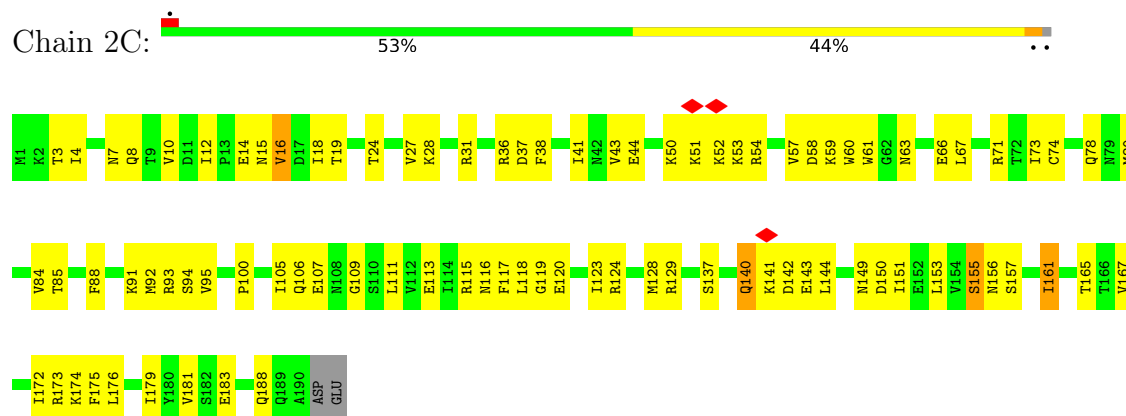
Chain 1G: 



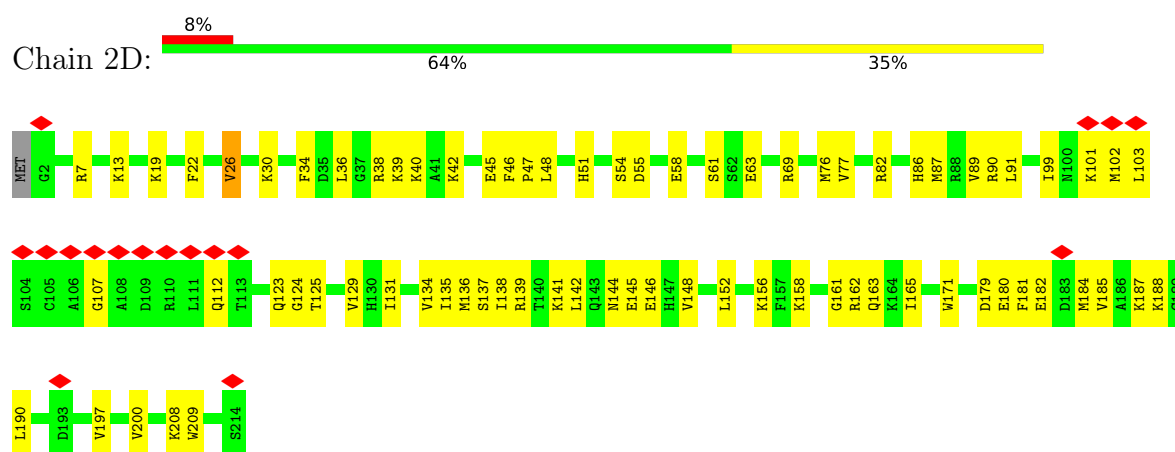
- Molecule 10: 60S ribosomal protein L7a



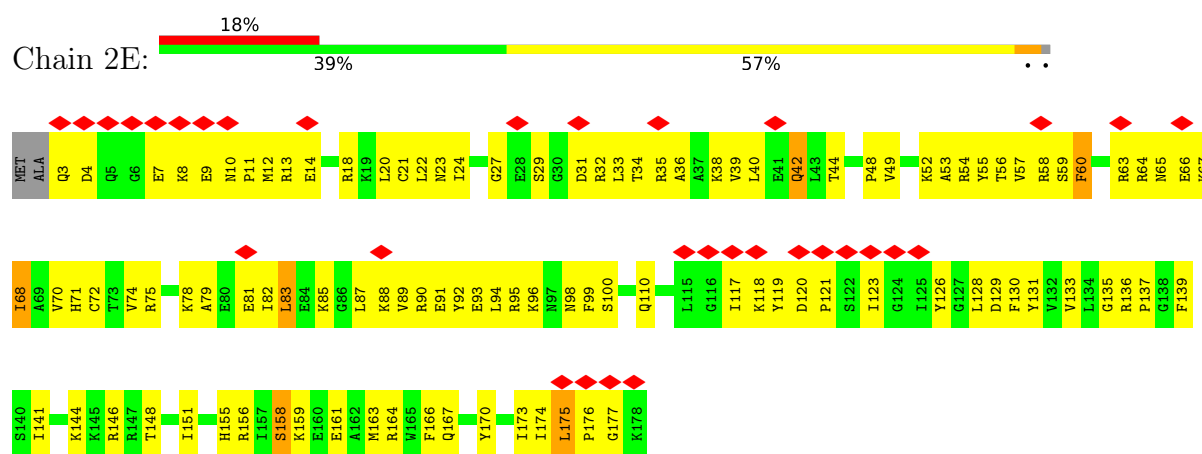
- Molecule 11: 60S ribosomal protein L9



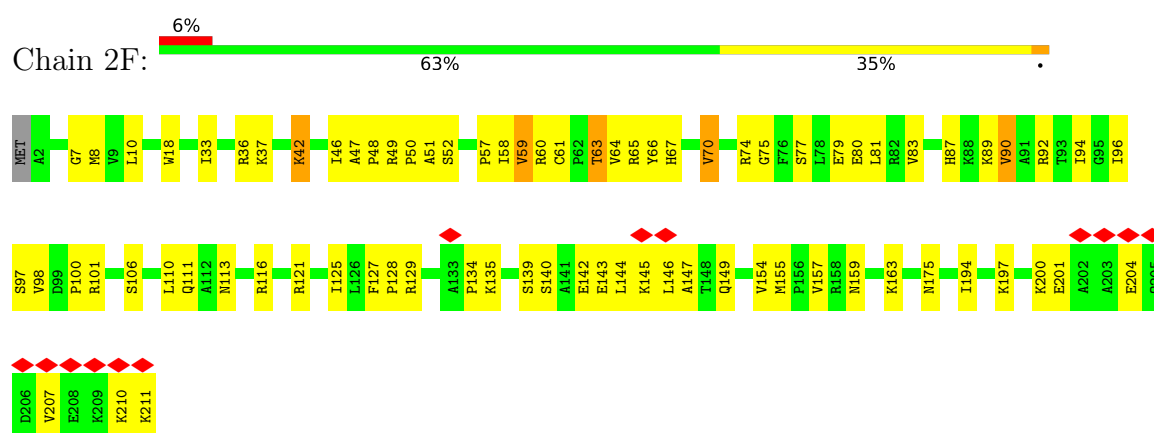
- Molecule 12: 60S ribosomal protein L10-like



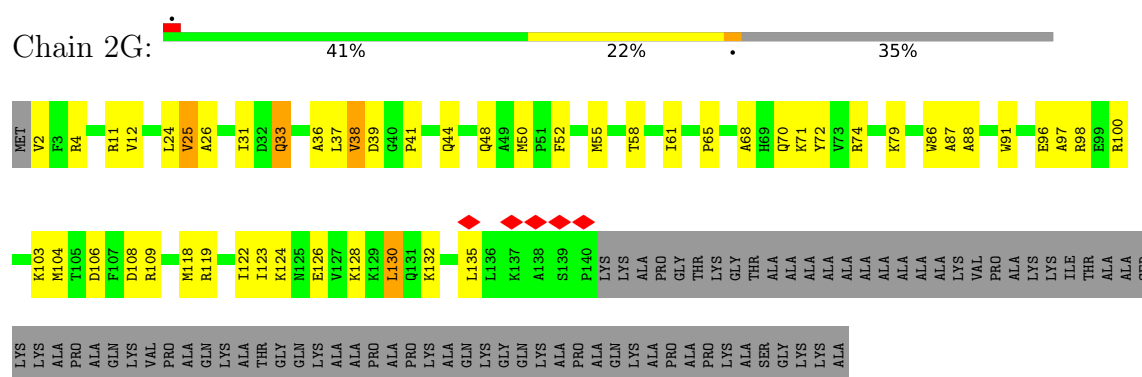
- Molecule 13: 60S ribosomal protein L11



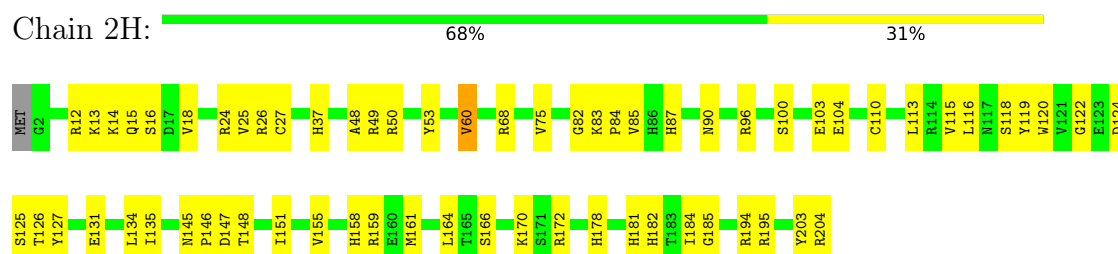
• Molecule 14: 60S ribosomal protein L13



• Molecule 15: 60S ribosomal protein L14



• Molecule 16: 60S ribosomal protein L15



Chain 2I: 

[illegible]

Chain 2K:  74% 24%

Chain 2L:

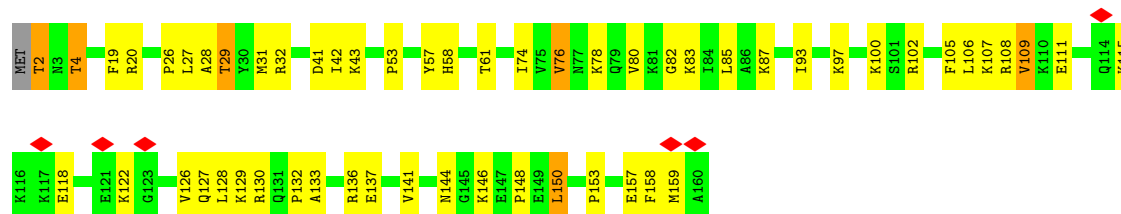
| Amino Acid | Count | Percentage |
|------------|-------|------------|
| Met        | 1     | 0.1%       |
| S2         | 1     | 0.1%       |
| M3         | 1     | 0.1%       |
| L4         | 1     | 0.1%       |
| Q7         | 1     | 0.1%       |
| K20        | 1     | 0.1%       |
| K21        | 1     | 0.1%       |
| L24        | 1     | 0.1%       |
| E28        | 1     | 0.1%       |
| A33        | 1     | 0.1%       |
| R38        | 1     | 0.1%       |
| L44        | 1     | 0.1%       |
| D47        | 1     | 0.1%       |
| G48        | 1     | 0.1%       |
| L49        | 1     | 0.1%       |
| I50        | 1     | 0.1%       |
| V55        | 1     | 0.1%       |
| T56        | 1     | 0.1%       |
| V57        | 1     | 0.1%       |
| H58        | 1     | 0.1%       |
| R64        | 1     | 0.1%       |
| T67        | 1     | 0.1%       |
| R71        | 1     | 0.1%       |
| G77        | 1     | 0.1%       |
| I78        | 1     | 0.1%       |
| G79        | 1     | 0.1%       |
| K80        | 1     | 0.1%       |
| R81        | 1     | 0.1%       |
| T84        | 1     | 0.1%       |
| A87        | 1     | 0.1%       |
| R88        | 1     | 0.1%       |
| V93        | 1     | 0.1%       |
| T94        | 1     | 0.1%       |
| H95        | 1     | 0.1%       |
| M96        | 1     | 0.1%       |
| M99        | 1     | 0.1%       |
| L103       | 1     | 0.1%       |
| R108       | 1     | 0.1%       |
| S112       | 1     | 0.1%       |
| K113       | 1     | 0.1%       |
| K114       | 1     | 0.1%       |
| Y124       | 1     | 0.1%       |
| I137       | 1     | 0.1%       |
| K144       | 1     | 0.1%       |
| K149       | 1     | 0.1%       |
| L154       | 1     | 0.1%       |
| D157       | 1     | 0.1%       |
| Q158       | 1     | 0.1%       |
| A159       | 1     | 0.1%       |
| E160       | 1     | 0.1%       |
| A161       | 1     | 0.1%       |
| R162       | 1     | 0.1%       |
| R163       | 1     | 0.1%       |
| S164       | 1     | 0.1%       |
| K165       | 1     | 0.1%       |
| T166       | 1     | 0.1%       |
| K167       | 1     | 0.1%       |
| E168       | 1     | 0.1%       |
| A169       | 1     | 0.1%       |
| R170       | 1     | 0.1%       |
| K171       | 1     | 0.1%       |
| R172       | 1     | 0.1%       |
| R173       | 1     | 0.1%       |
| E174       | 1     | 0.1%       |
| E175       | 1     | 0.1%       |
| R176       | 1     | 0.1%       |
| L177       | 1     | 0.1%       |
| Q178       | 1     | 0.1%       |
| A179       | 1     | 0.1%       |
| K180       | 1     | 0.1%       |
| K181       | 1     | 0.1%       |
| E182       | 1     | 0.1%       |
| E183       | 1     | 0.1%       |
| I184       | 1     | 0.1%       |
| I186       | 1     | 0.1%       |
| K186       | 1     | 0.1%       |
| T187       | 1     | 0.1%       |
| L188       | 1     | 0.1%       |
| SER        | 1     | 0.1%       |
| LYS        | 1     | 0.1%       |
| GLU        | 1     | 0.1%       |
| GLU        | 1     | 0.1%       |
| THR        | 1     | 0.1%       |
| LYS        | 1     | 0.1%       |

Chain 2M: 

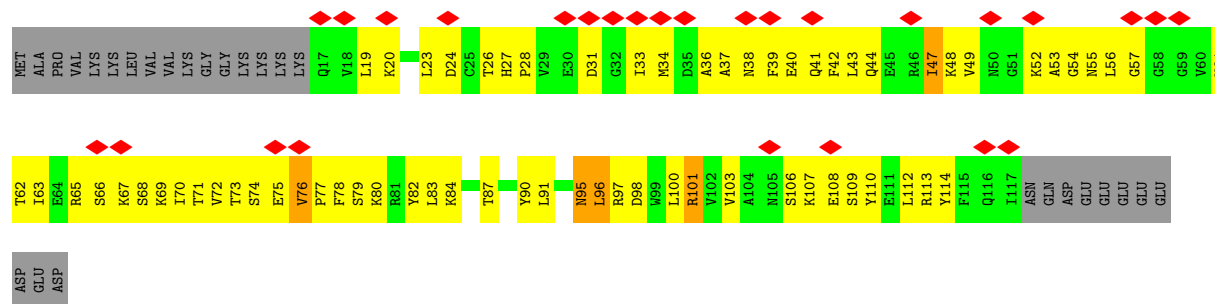




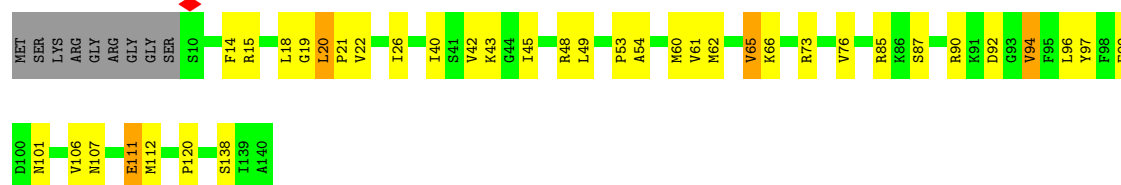
- Molecule 22: 60S ribosomal protein L21



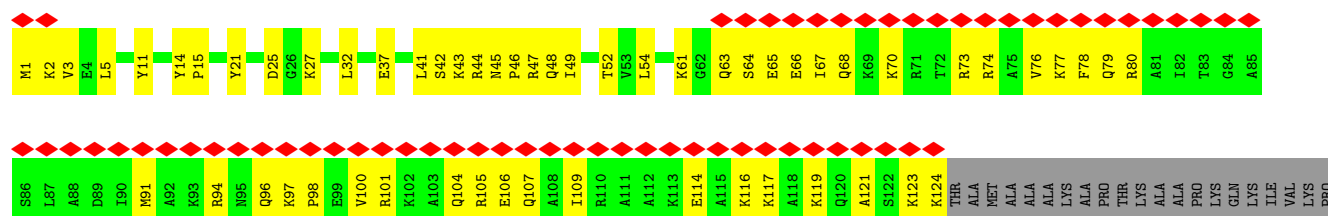
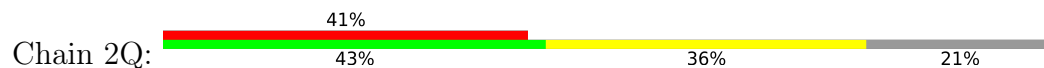
- Molecule 23: 60S ribosomal protein L22



- Molecule 24: 60S ribosomal protein L23



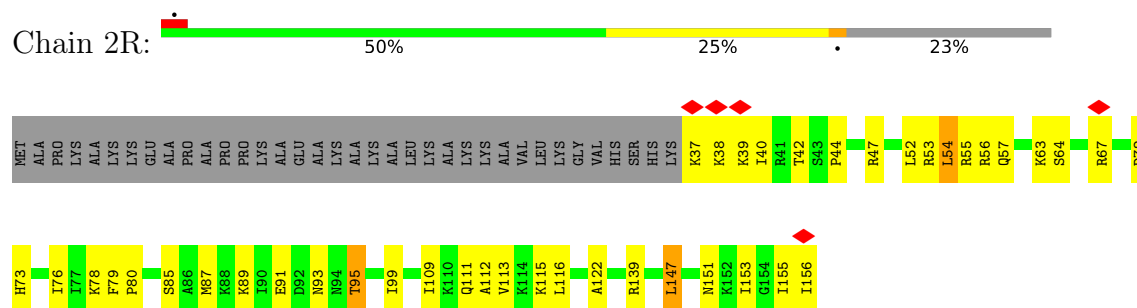
- Molecule 25: 60S ribosomal protein L24



VAL  
LYS  
VAL  
SER  
ALA  
PRO  
ARG  
VAL  
GLY  
LYS  
ARG

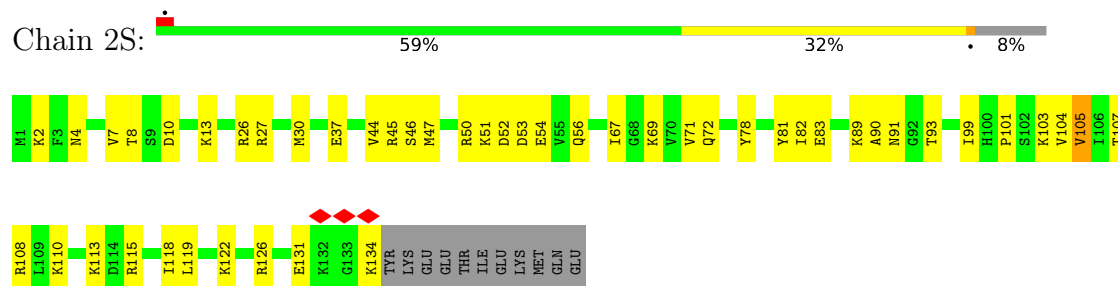
• Molecule 26: 60S ribosomal protein L23a

Chain 2R:



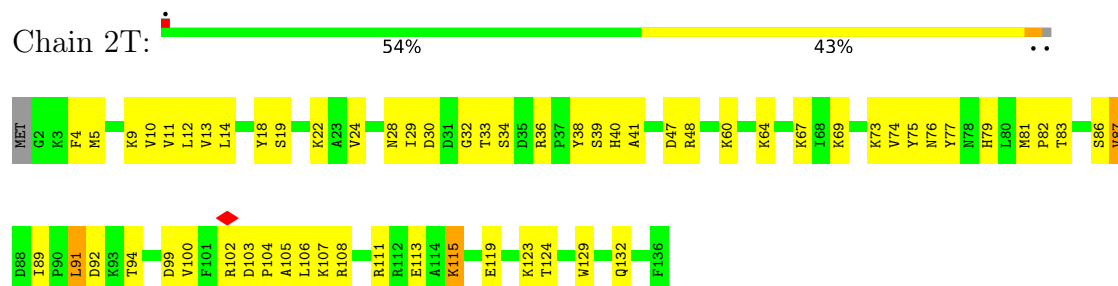
• Molecule 27: 60S ribosomal protein L26

Chain 2S:



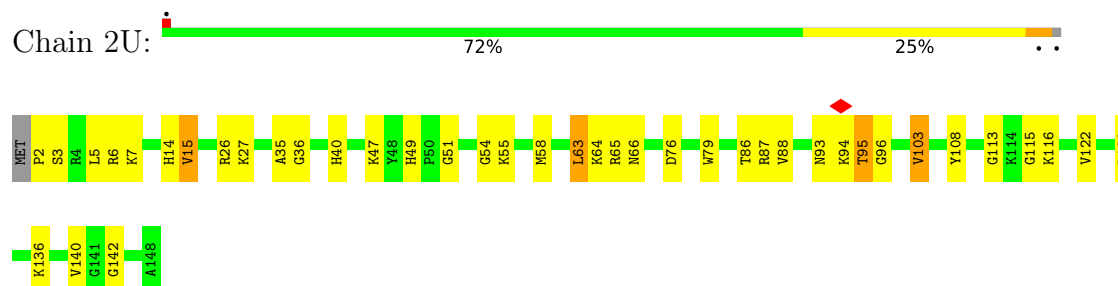
• Molecule 28: 60S ribosomal protein L27

Chain 2T:



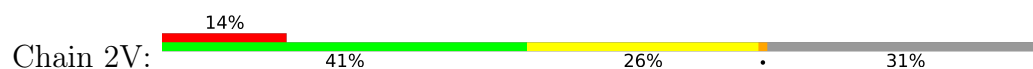
• Molecule 29: 60S ribosomal protein L27a

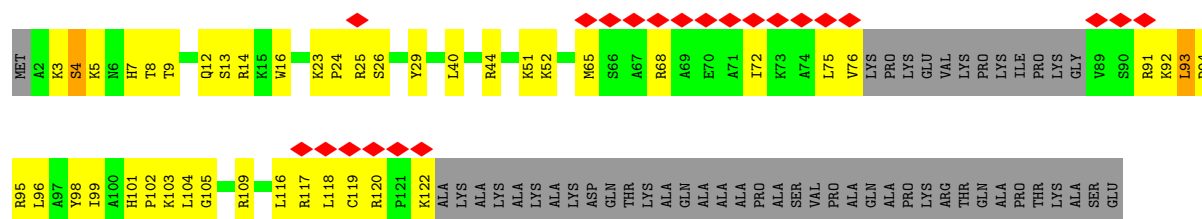
Chain 2U:



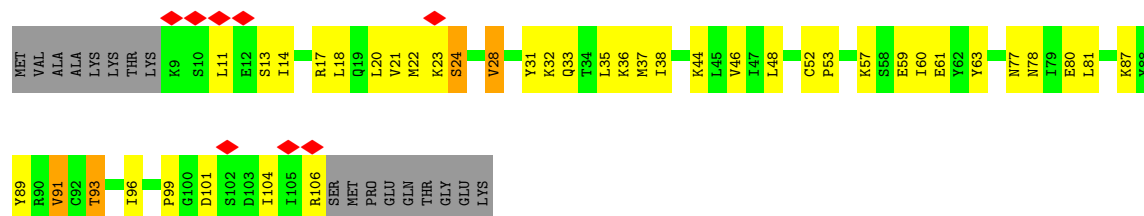
• Molecule 30: 60S ribosomal protein L29

Chain 2V:

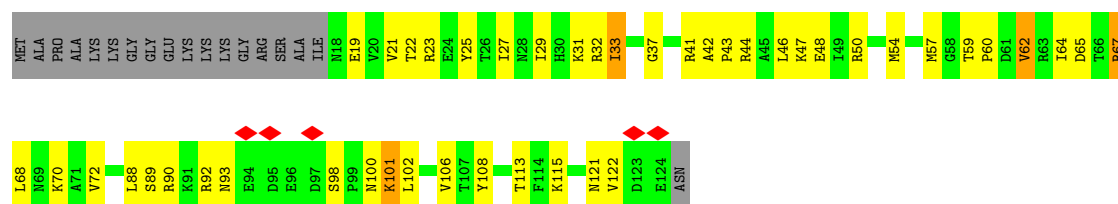




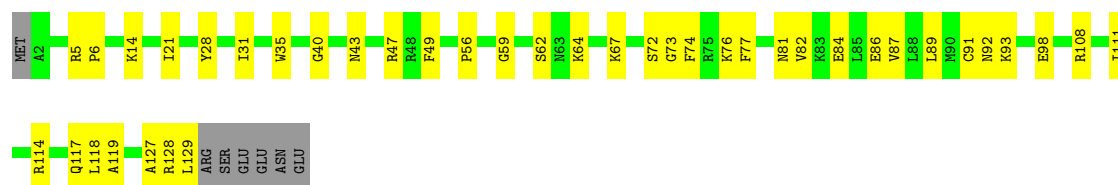
• Molecule 31: 60S ribosomal protein L30



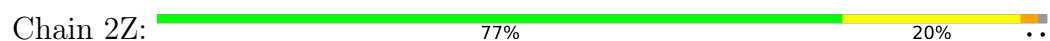
• Molecule 32: 60S ribosomal protein L31



• Molecule 33: 60S ribosomal protein L32

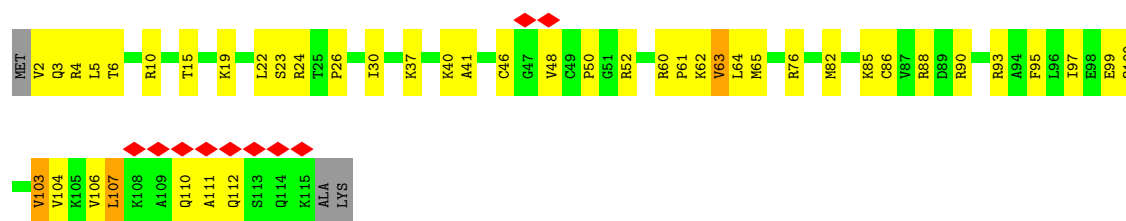


• Molecule 34: 60S ribosomal protein L35a

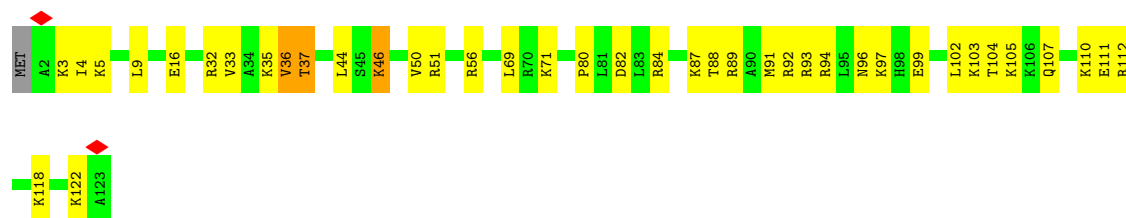


• Molecule 35: 60S ribosomal protein L34

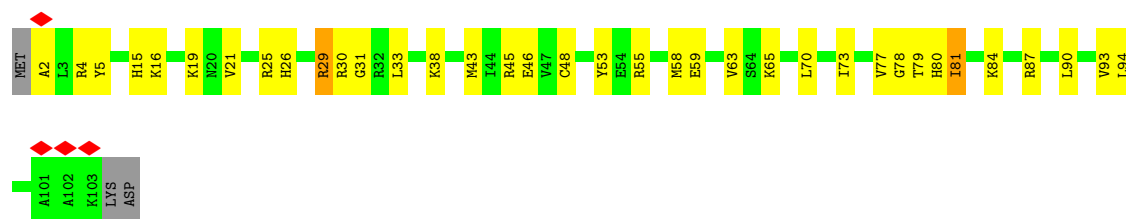




- Molecule 36: 60S ribosomal protein L35



- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



- Molecule 39: 60S ribosomal protein L38

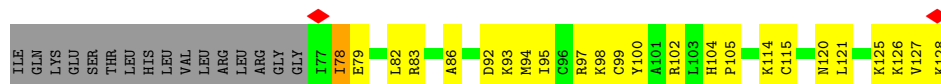
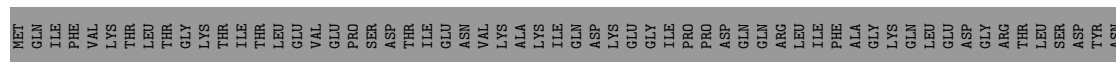


- Molecule 40: 60S ribosomal protein L39





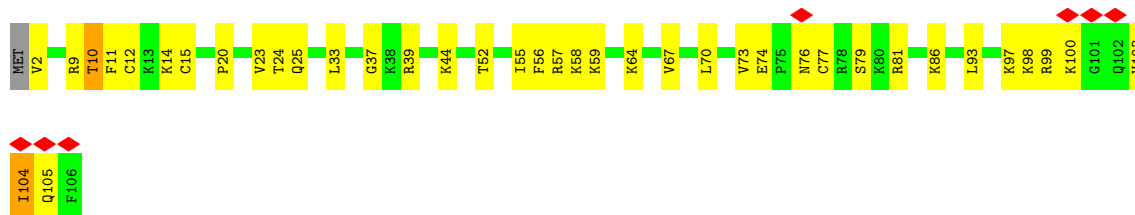
- Molecule 41: Large ribosomal subunit protein eL40



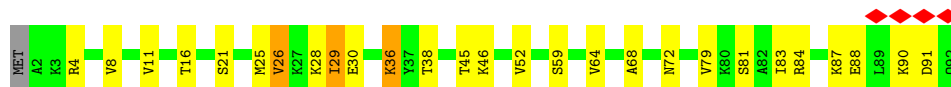
- Molecule 42: 60S ribosomal protein L41



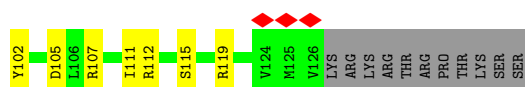
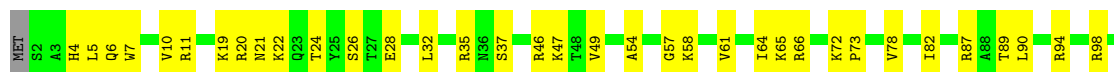
- Molecule 43: 60S ribosomal protein L36a



- Molecule 44: 60S ribosomal protein L37a

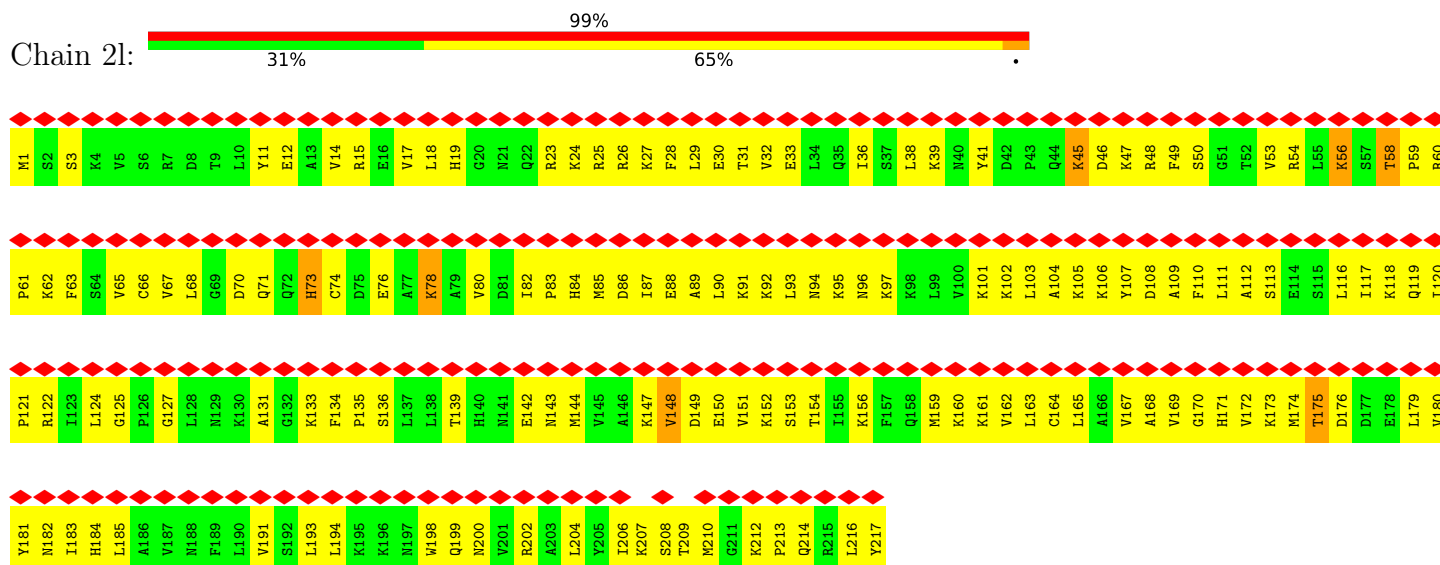


- Molecule 45: 60S ribosomal protein L28



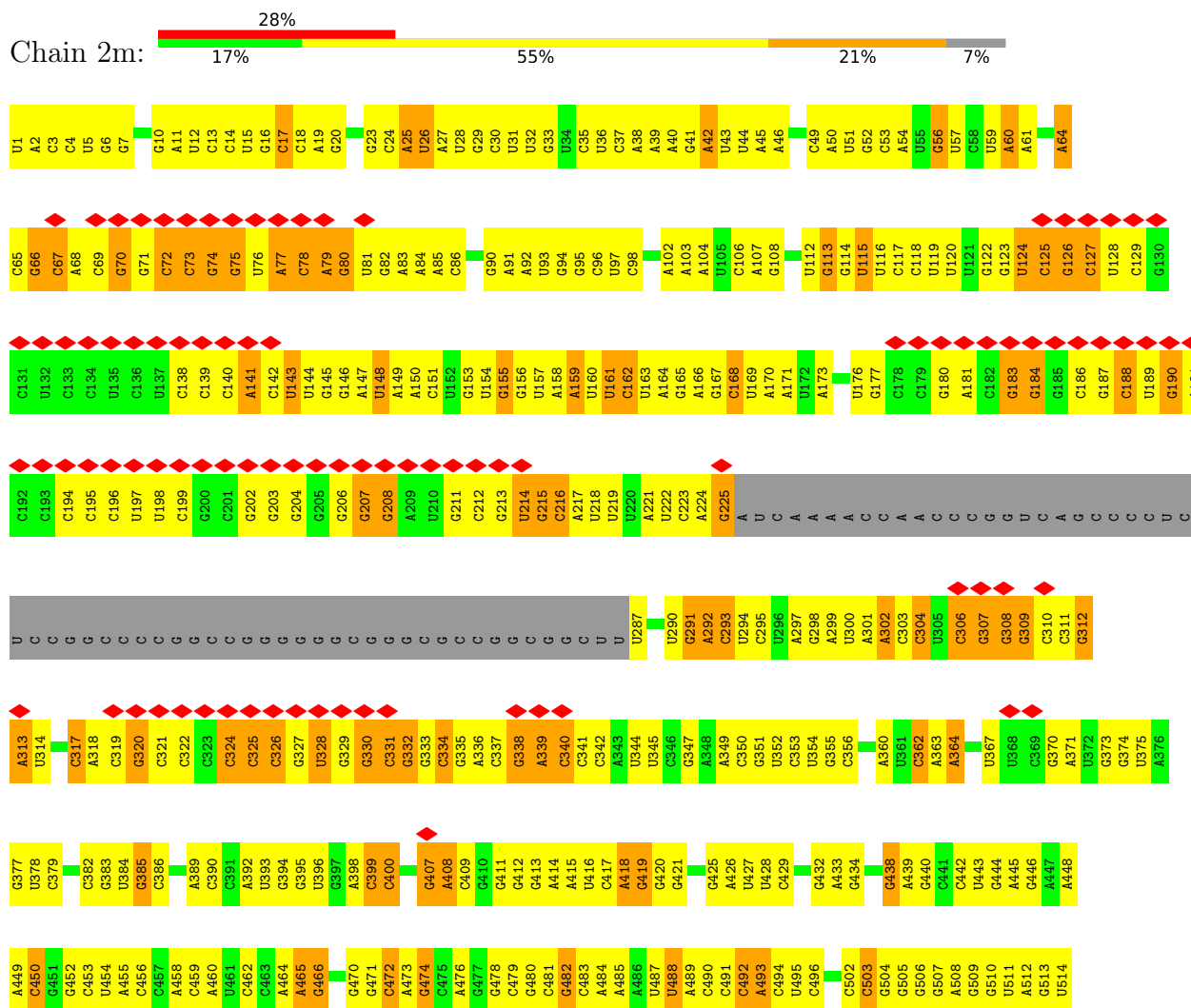
• Molecule 46: 60S ribosomal protein L10a

Chain 2l:

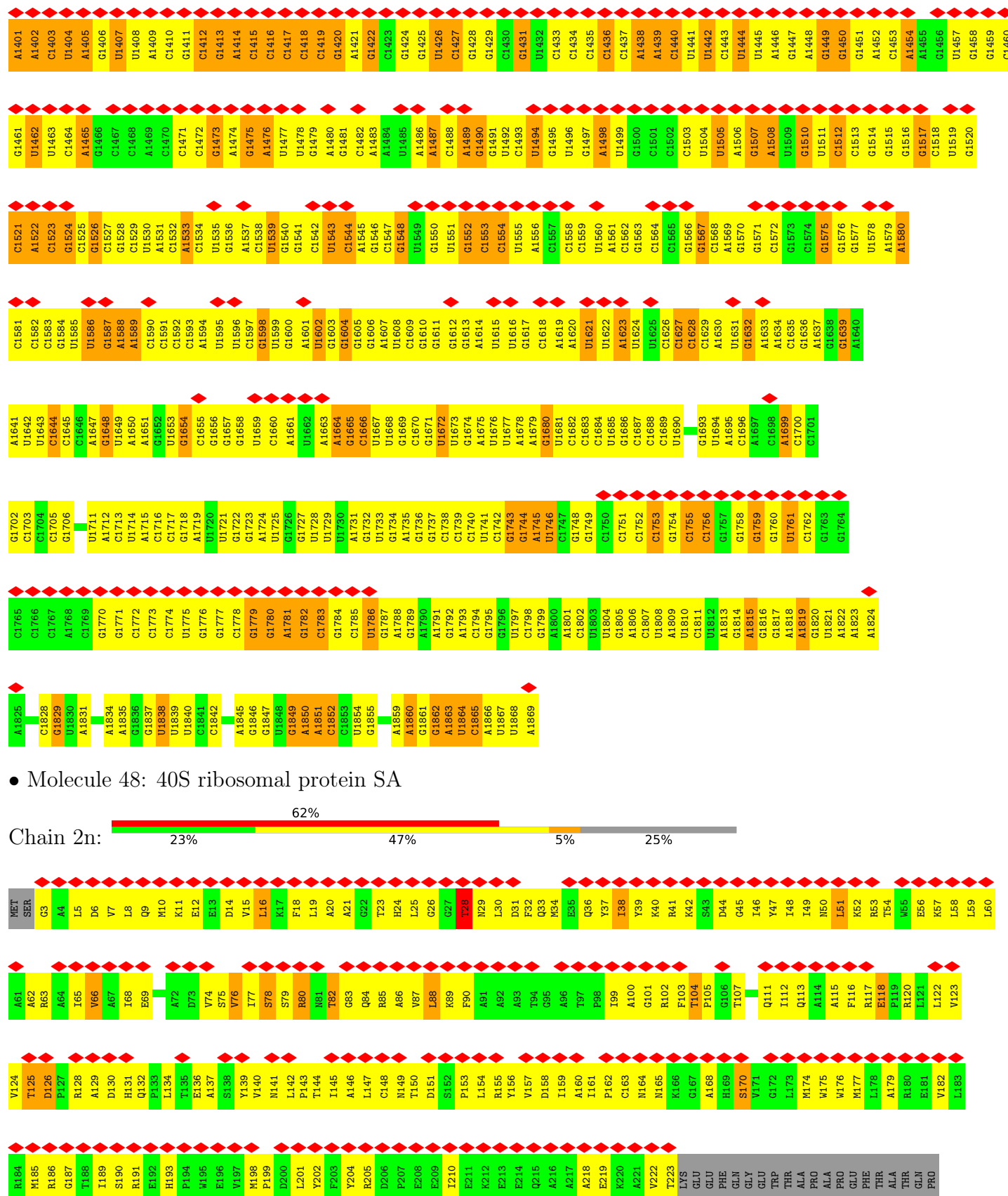


• Molecule 47: 18S ribosomal RNA

Chain 2m:

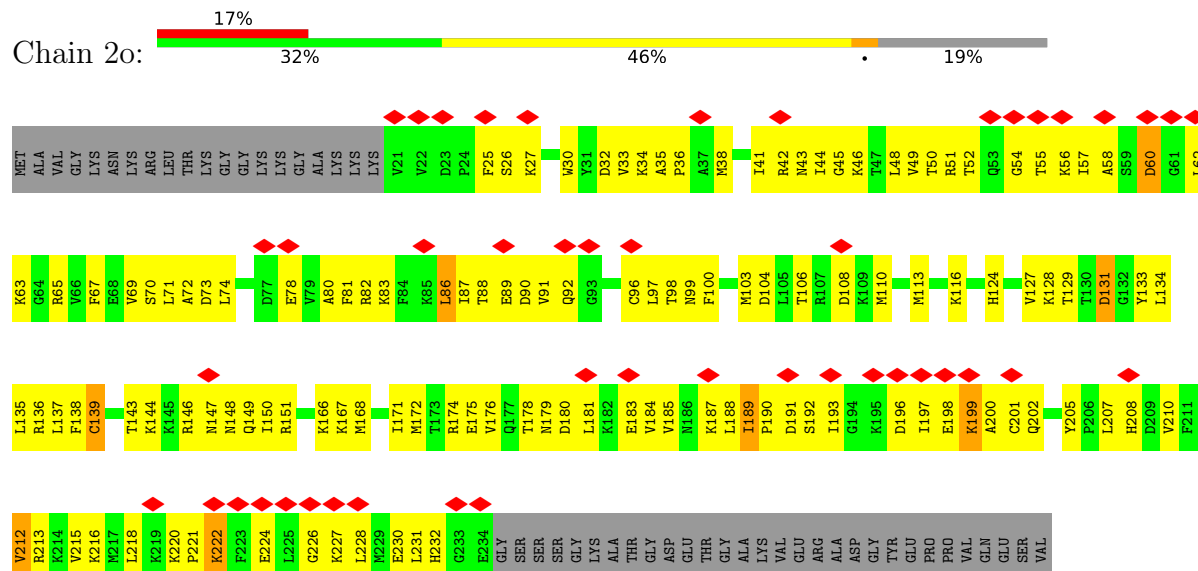




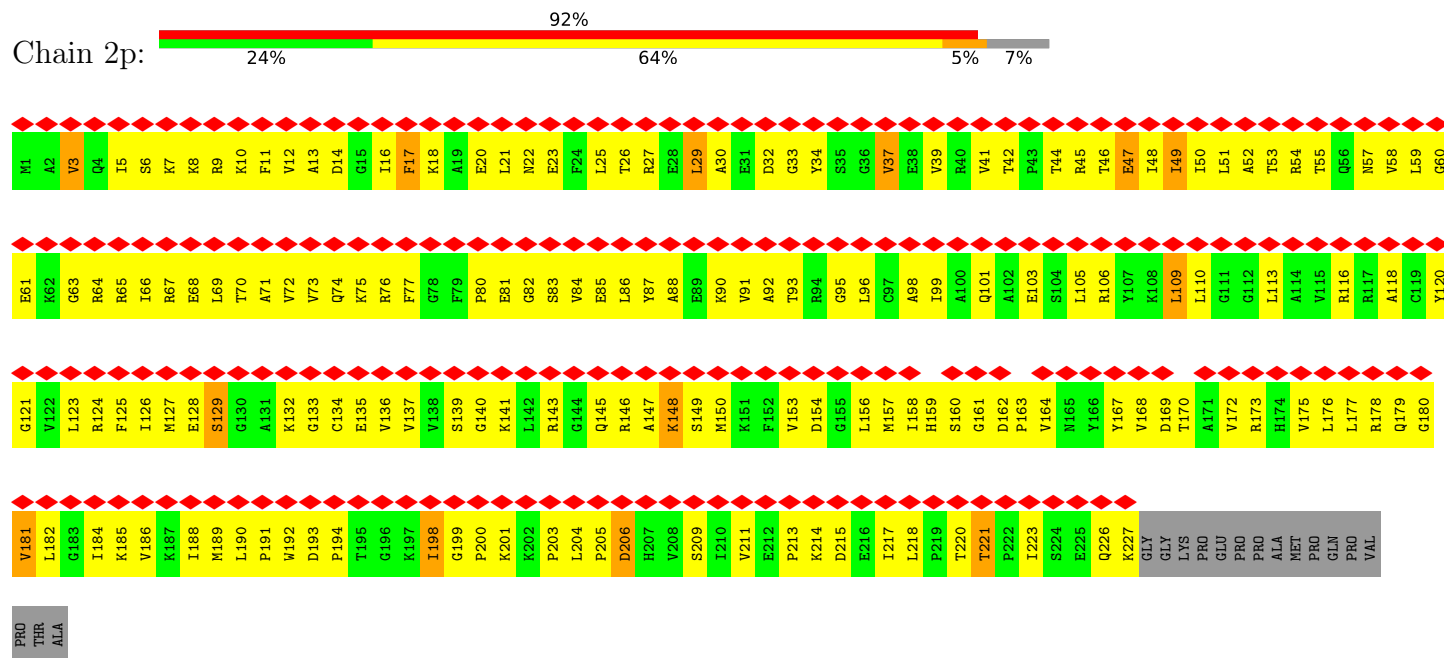




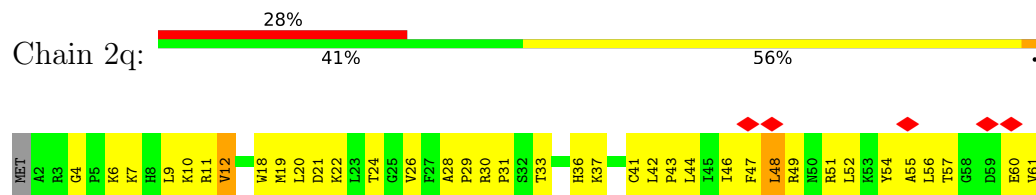
- Molecule 49: 40S ribosomal protein S3a

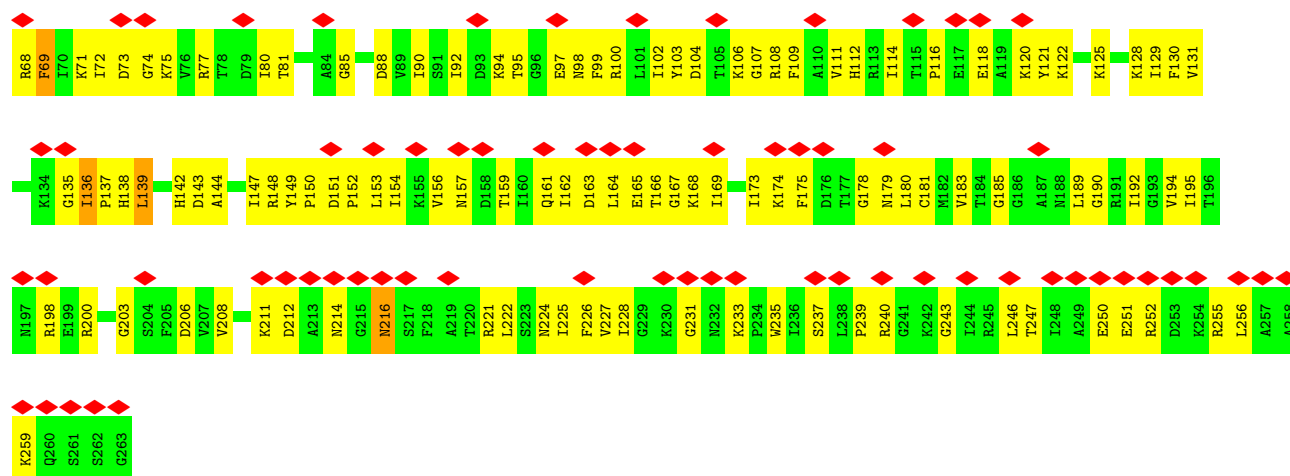


- Molecule 50: 40S ribosomal protein S3

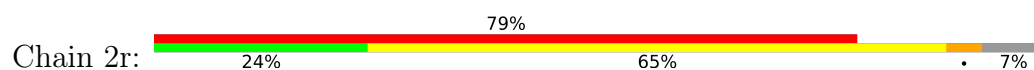


- Molecule 51: 40S ribosomal protein S4, X isoform





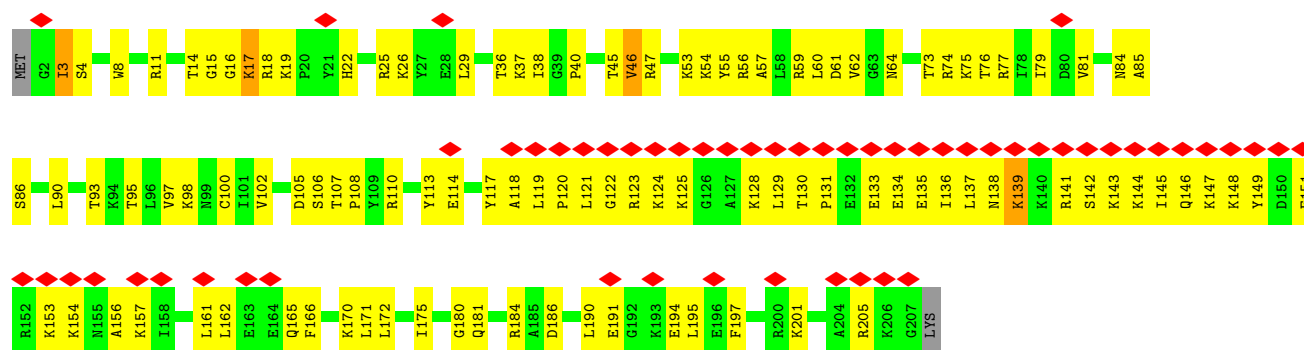
• Molecule 52: 40S ribosomal protein S5



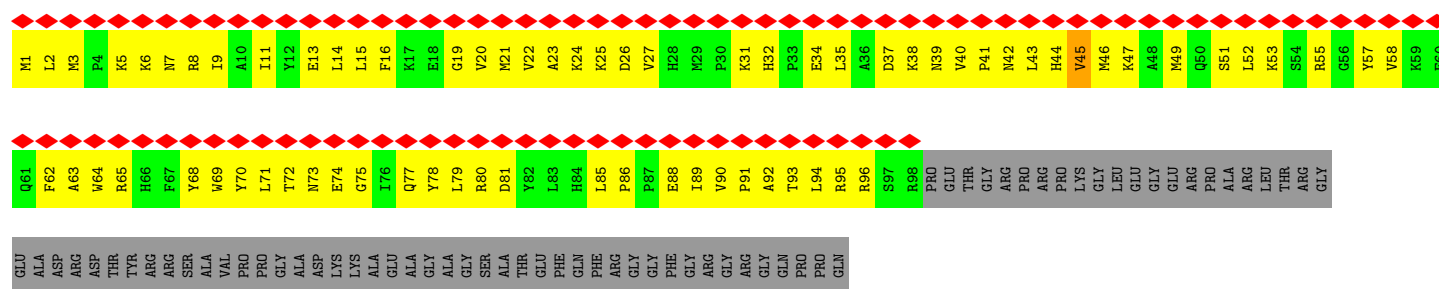
• Molecule 53: 40S ribosomal protein S7



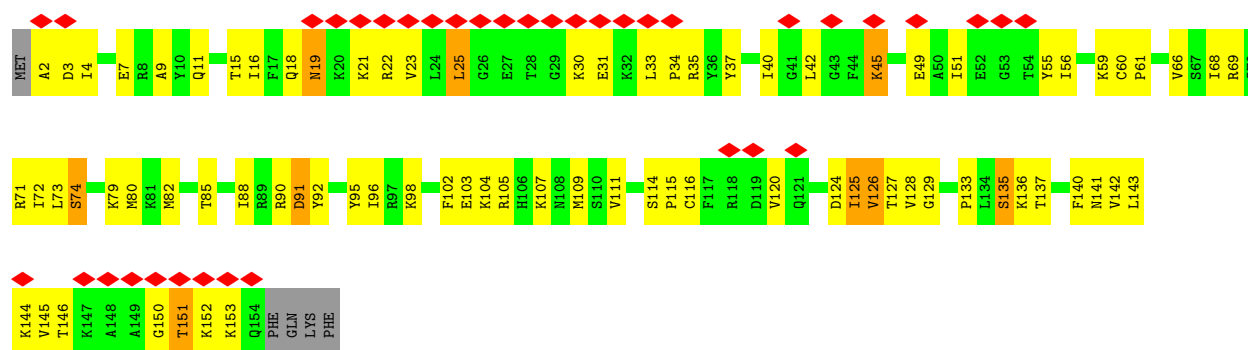
Chain 2t:  27% 47% 50%



Chain 2u:  16% 59% 43% 41%

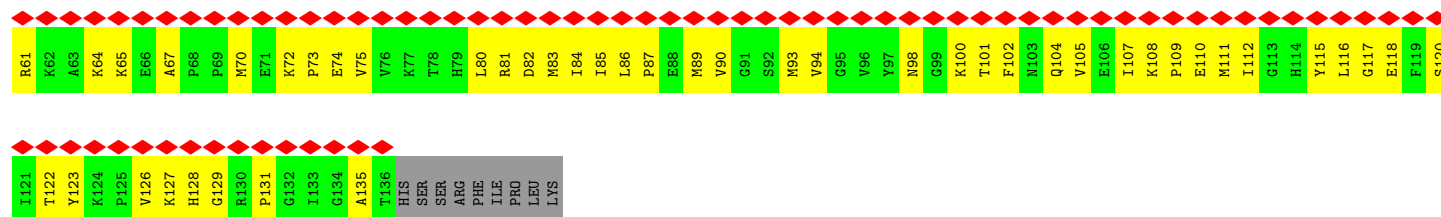


Chain 2v: 

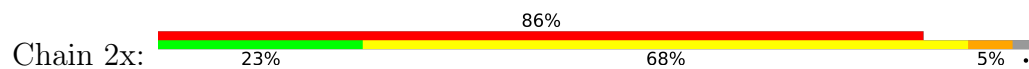


Chain 2w:  32% 88% 54% 12%





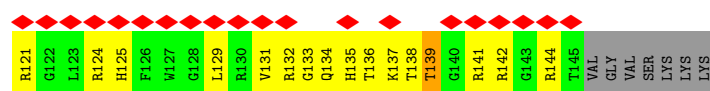
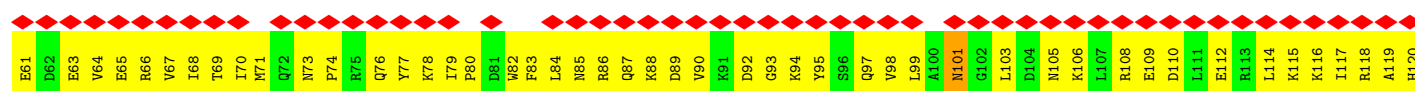
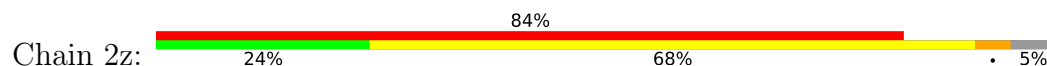
• Molecule 58: 40S ribosomal protein S16



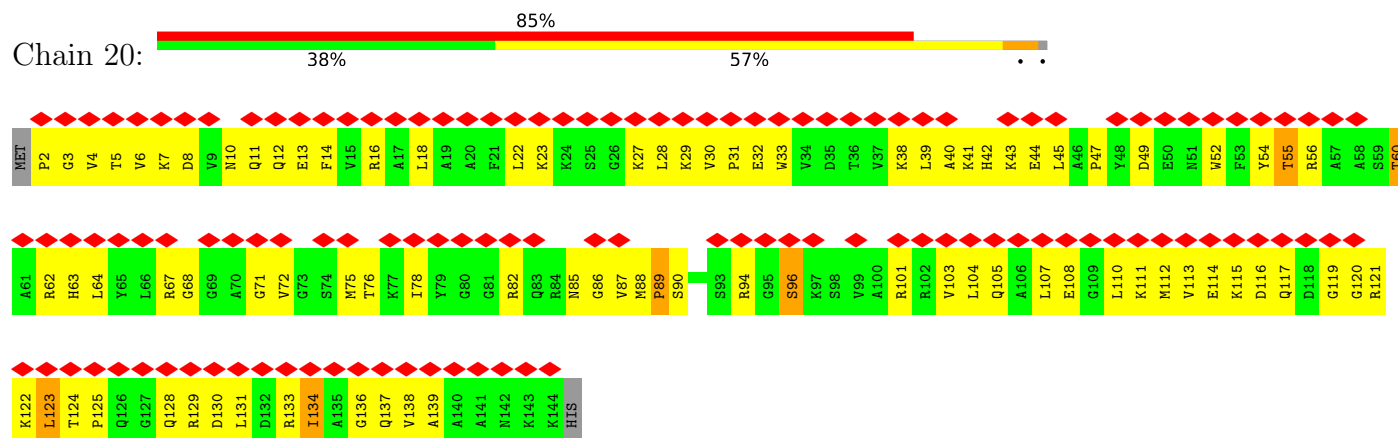
• Molecule 59: 40S ribosomal protein S17



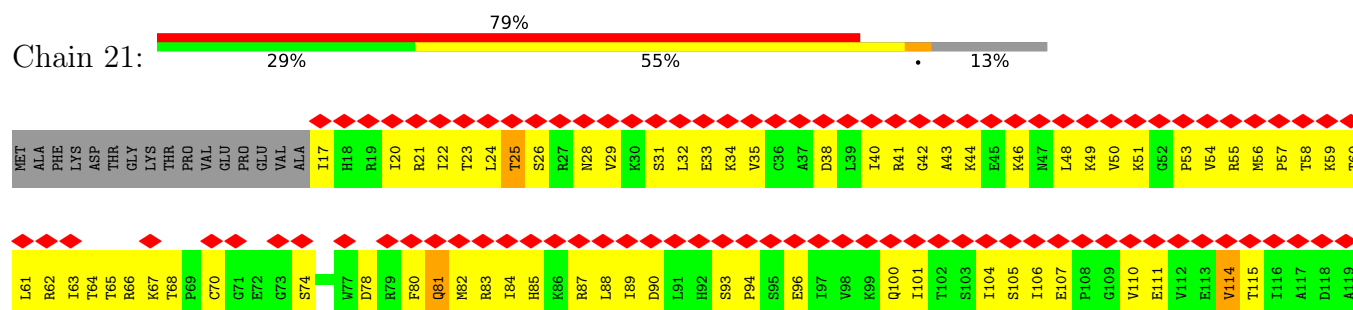
• Molecule 60: 40S ribosomal protein S18



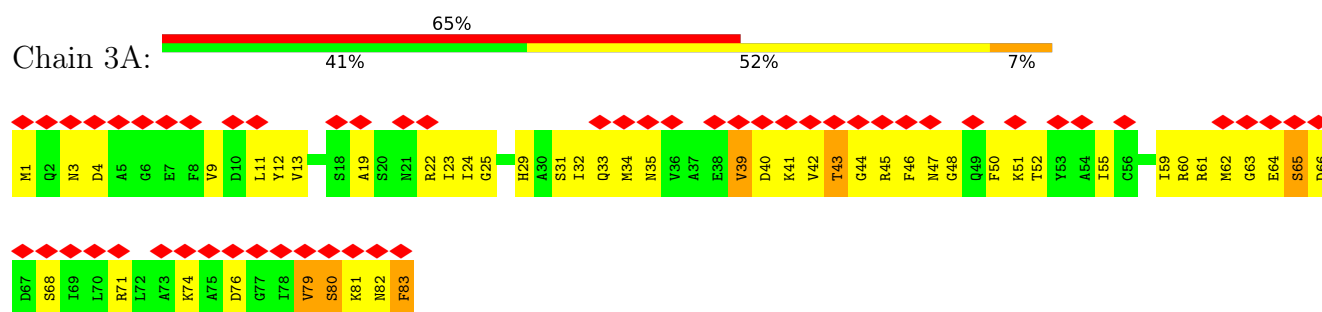
- Molecule 61: 40S ribosomal protein S19



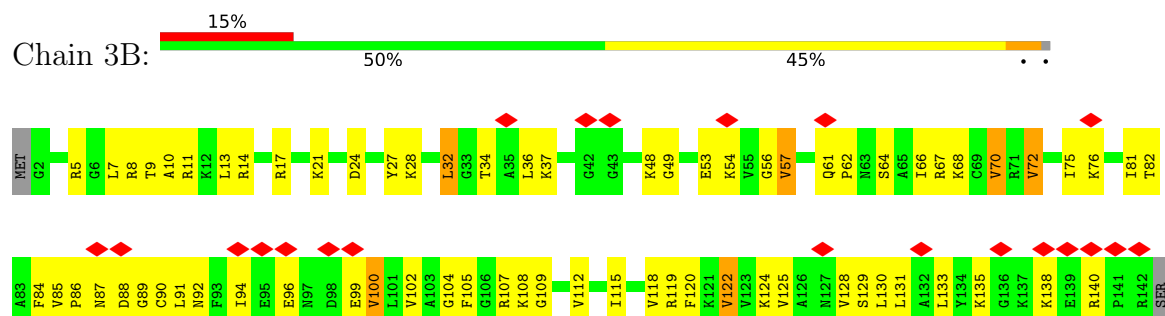
- Molecule 62: 40S ribosomal protein S20



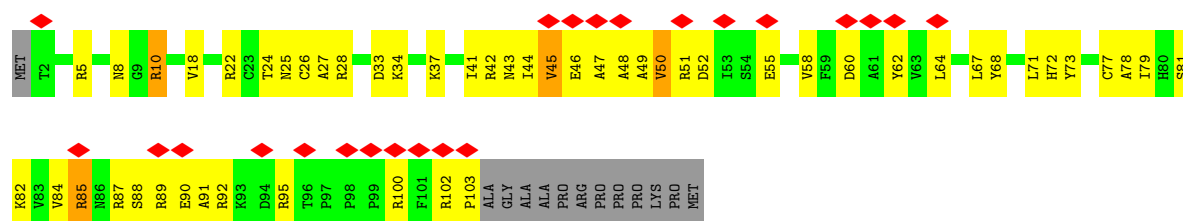
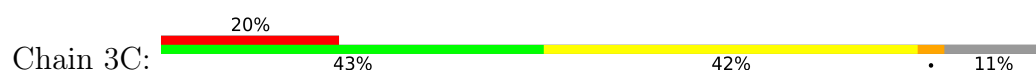
- Molecule 63: 40S ribosomal protein S21



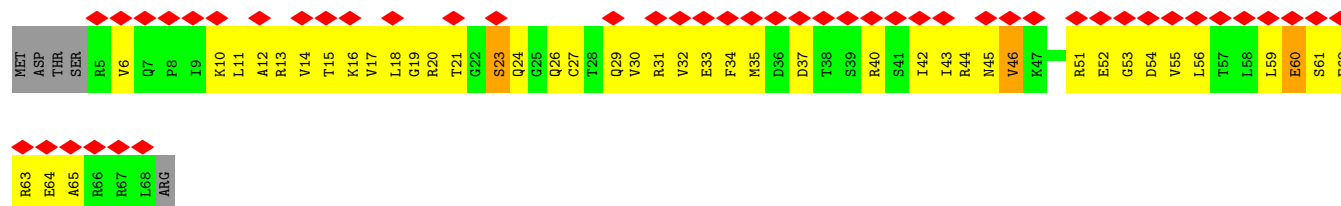
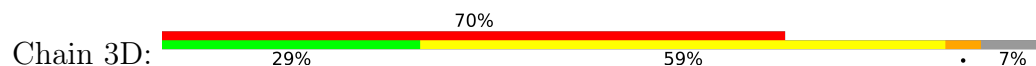
- Molecule 64: 40S ribosomal protein S23



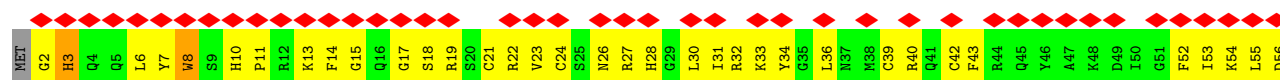
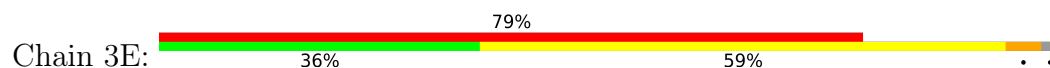
- Molecule 65: 40S ribosomal protein S26



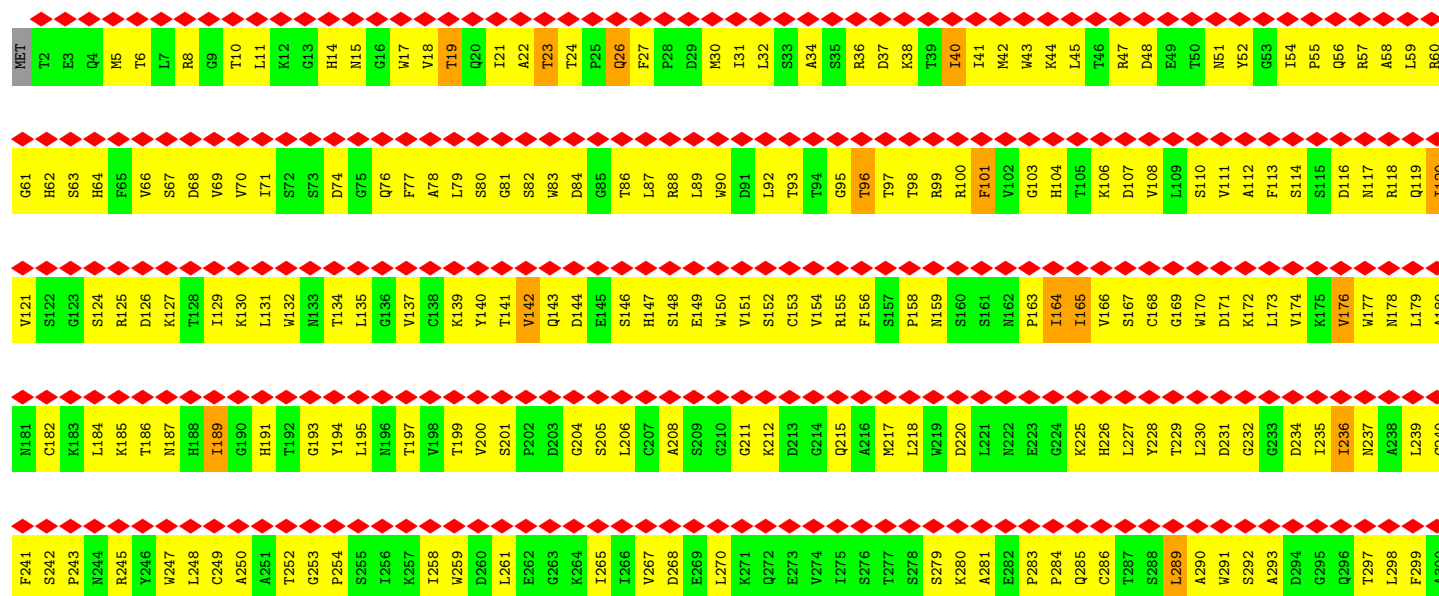
- Molecule 66: 40S ribosomal protein S28

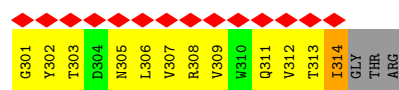


- Molecule 67: 40S ribosomal protein S29

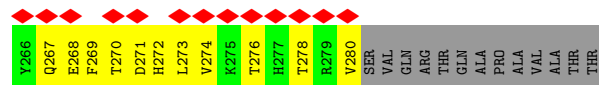
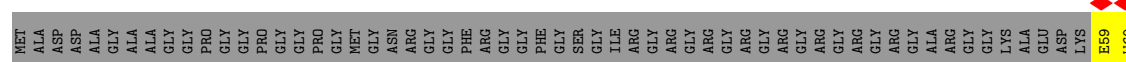


- Molecule 68: Receptor of activated protein C kinase 1

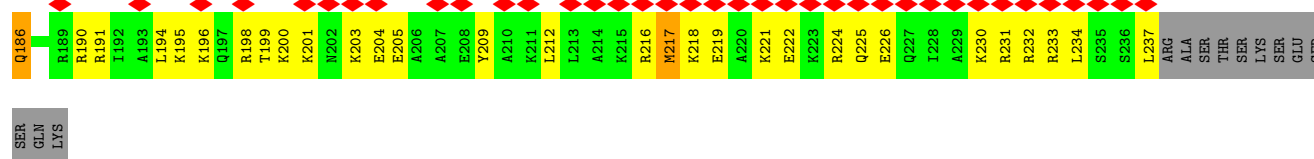
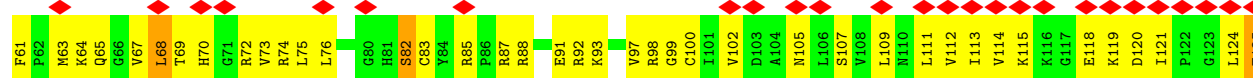
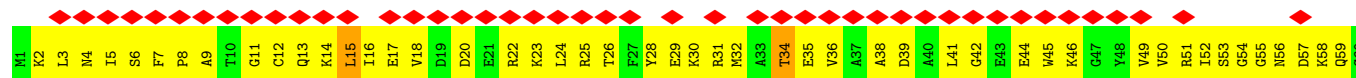




• Molecule 69: 40S ribosomal protein S2

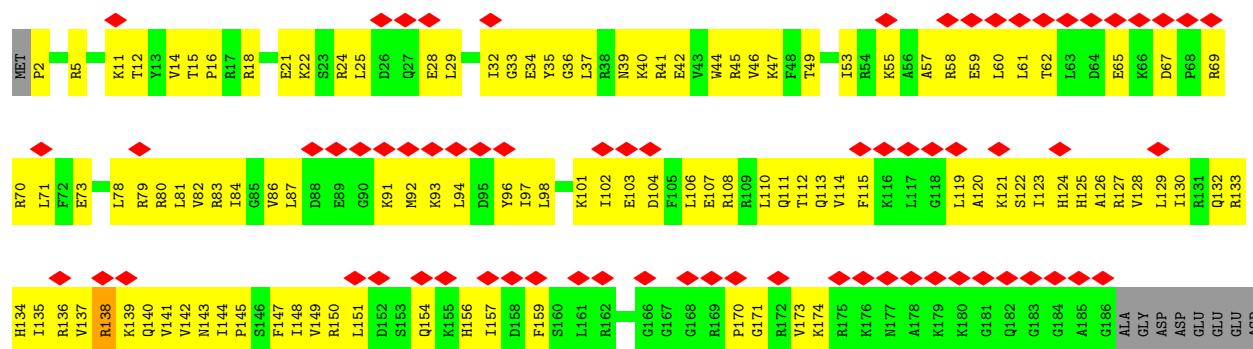


• Molecule 70: 40S ribosomal protein S6

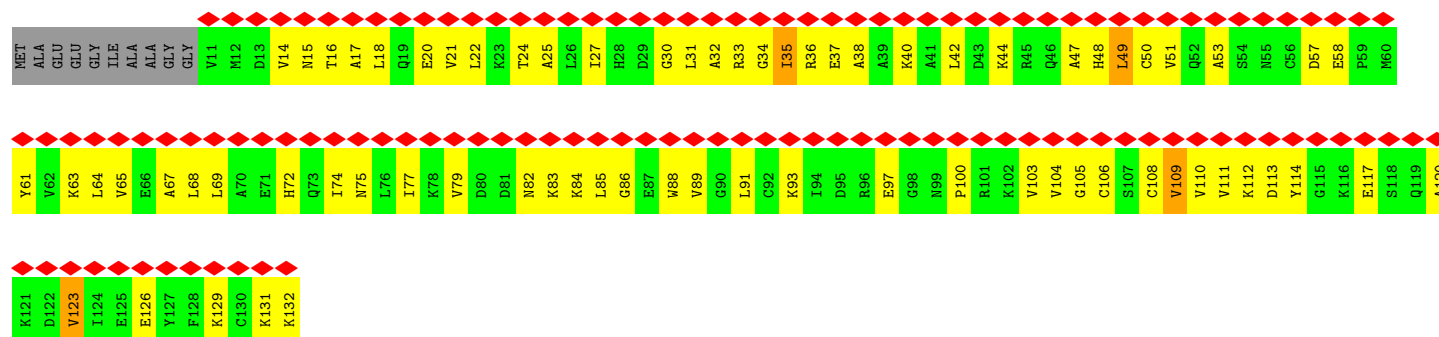
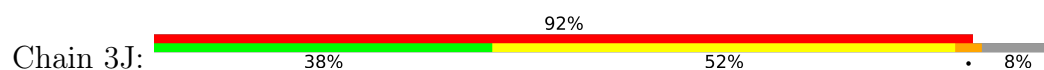


• Molecule 71: 40S ribosomal protein S9

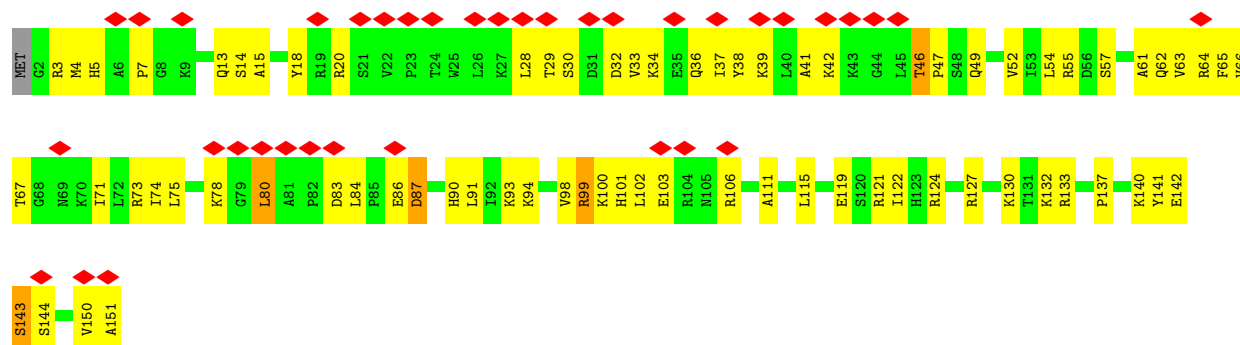




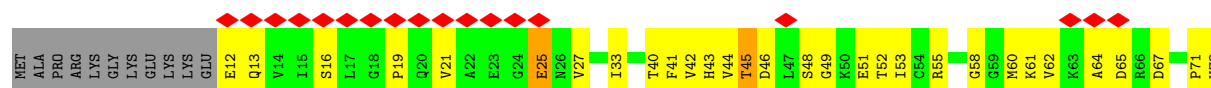
• Molecule 72: 40S ribosomal protein S12



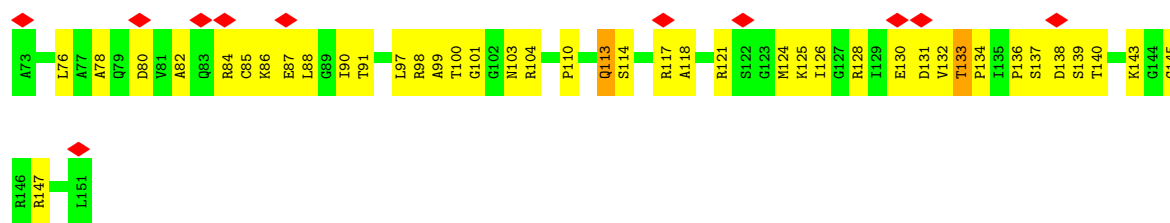
• Molecule 73: 40S ribosomal protein S13



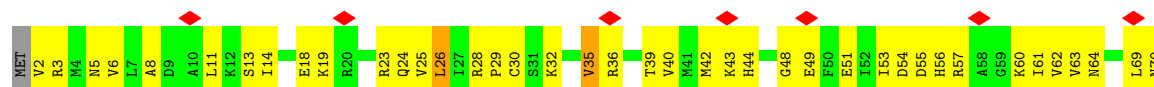
• Molecule 74: 40S ribosomal protein S14



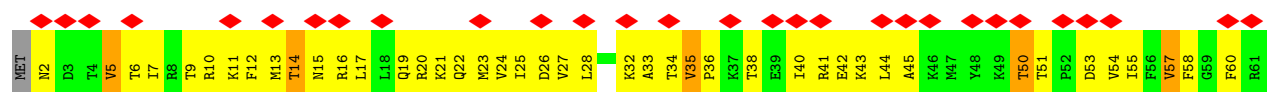




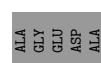
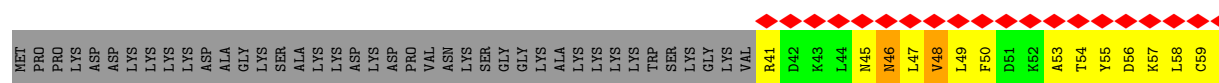
- Molecule 75: 40S ribosomal protein S15a



- Molecule 76: 40S ribosomal protein S24

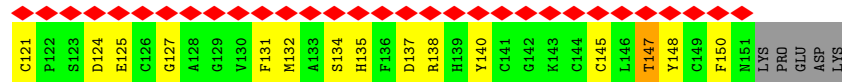


- Molecule 77: 40S ribosomal protein S25



- Molecule 78: 40S ribosomal protein S27





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 28291                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL CRYO ARM 300                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 1100                                    | Depositor |
| Maximum defocus (nm)                 | 2300                                    | Depositor |
| Magnification                        | 60000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.089                                   | Depositor |
| Minimum map value                    | -0.025                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.013                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 504.32, 504.32, 504.32                  | wwPDB     |
| Map dimensions                       | 640, 640, 640                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.788, 0.788, 0.788                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, MG, ZN, 84D

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | 1A    | 0.10         | 0/89127     | 0.25        | 0/139035      |
| 2   | 1B    | 0.09         | 0/2858      | 0.24        | 0/4455        |
| 3   | 1C    | 0.09         | 0/3696      | 0.25        | 0/5758        |
| 4   | 1D    | 0.09         | 0/1936      | 0.26        | 0/2596        |
| 5   | 1E    | 0.09         | 0/3306      | 0.25        | 0/4424        |
| 6   | 1F    | 0.11         | 0/2981      | 0.29        | 0/4002        |
| 7   | 1G    | 0.10         | 0/2428      | 0.29        | 0/3252        |
| 8   | 1H    | 0.10         | 0/1942      | 0.27        | 0/2606        |
| 9   | 2A    | 0.11         | 0/1916      | 0.28        | 0/2553        |
| 10  | 2B    | 0.10         | 0/1971      | 0.27        | 0/2651        |
| 11  | 2C    | 0.09         | 0/1537      | 0.27        | 0/2066        |
| 12  | 2D    | 0.09         | 0/1751      | 0.24        | 0/2340        |
| 13  | 2E    | 0.09         | 0/1433      | 0.29        | 0/1915        |
| 14  | 2F    | 0.11         | 0/1732      | 0.27        | 0/2315        |
| 15  | 2G    | 0.11         | 0/1161      | 0.29        | 0/1554        |
| 16  | 2H    | 0.10         | 0/1746      | 0.26        | 0/2338        |
| 17  | 2I    | 0.11         | 0/1682      | 0.25        | 0/2250        |
| 18  | 2J    | 0.10         | 0/1268      | 0.27        | 0/1701        |
| 19  | 2K    | 0.10         | 0/1537      | 0.25        | 0/2052        |
| 20  | 2L    | 0.09         | 0/1582      | 0.24        | 1/2091 (0.0%) |
| 21  | 2M    | 0.11         | 0/1493      | 0.30        | 0/2003        |
| 22  | 2N    | 0.10         | 0/1326      | 0.24        | 0/1770        |
| 23  | 2O    | 0.10         | 0/839       | 0.30        | 0/1126        |
| 24  | 2P    | 0.10         | 0/993       | 0.25        | 0/1332        |
| 25  | 2Q    | 0.09         | 0/1030      | 0.26        | 0/1364        |
| 26  | 2R    | 0.09         | 0/1002      | 0.24        | 0/1345        |
| 27  | 2S    | 0.10         | 0/1132      | 0.26        | 0/1504        |
| 28  | 2T    | 0.10         | 0/1130      | 0.28        | 0/1507        |
| 29  | 2U    | 0.09         | 0/1191      | 0.23        | 0/1591        |
| 30  | 2V    | 0.09         | 0/895       | 0.25        | 0/1182        |
| 31  | 2W    | 0.10         | 0/774       | 0.24        | 0/1038        |
| 32  | 2X    | 0.10         | 0/903       | 0.26        | 0/1216        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 33  | 2Y    | 0.10         | 0/1071  | 0.26        | 0/1429        |
| 34  | 2Z    | 0.10         | 0/895   | 0.28        | 0/1198        |
| 35  | 2a    | 0.09         | 0/916   | 0.25        | 0/1220        |
| 36  | 2b    | 0.08         | 0/1023  | 0.20        | 0/1351        |
| 37  | 2c    | 0.08         | 0/843   | 0.21        | 0/1115        |
| 38  | 2d    | 0.10         | 0/731   | 0.27        | 0/966         |
| 39  | 2e    | 0.10         | 0/575   | 0.26        | 0/761         |
| 40  | 2f    | 0.10         | 0/454   | 0.22        | 0/599         |
| 41  | 2g    | 0.10         | 0/425   | 0.26        | 0/561         |
| 42  | 2h    | 0.08         | 0/231   | 0.15        | 0/294         |
| 43  | 2i    | 0.09         | 0/887   | 0.25        | 0/1170        |
| 44  | 2j    | 0.08         | 0/718   | 0.22        | 0/953         |
| 45  | 2k    | 0.11         | 0/1017  | 0.25        | 0/1364        |
| 46  | 2l    | 0.09         | 0/1768  | 0.29        | 0/2371        |
| 47  | 2m    | 0.08         | 0/41243 | 0.22        | 0/64257       |
| 48  | 2n    | 0.08         | 0/1778  | 0.26        | 0/2416        |
| 49  | 2o    | 0.08         | 0/1765  | 0.24        | 0/2362        |
| 50  | 2p    | 0.10         | 0/1793  | 0.29        | 0/2414        |
| 51  | 2q    | 0.08         | 0/2118  | 0.26        | 0/2849        |
| 52  | 2r    | 0.08         | 0/1516  | 0.26        | 0/2037        |
| 53  | 2s    | 0.11         | 0/1519  | 0.28        | 0/2033        |
| 54  | 2t    | 0.09         | 0/1715  | 0.25        | 0/2287        |
| 55  | 2u    | 0.09         | 0/851   | 0.27        | 0/1147        |
| 56  | 2v    | 0.08         | 0/1268  | 0.27        | 0/1696        |
| 57  | 2w    | 0.08         | 0/1065  | 0.23        | 0/1423        |
| 58  | 2x    | 0.12         | 0/1142  | 0.31        | 0/1528        |
| 59  | 2y    | 0.09         | 0/1105  | 0.29        | 0/1484        |
| 60  | 2z    | 0.10         | 0/1216  | 0.28        | 0/1628        |
| 61  | 20    | 0.21         | 0/1131  | 0.40        | 2/1515 (0.1%) |
| 62  | 21    | 0.08         | 0/827   | 0.23        | 0/1110        |
| 63  | 3A    | 0.08         | 0/643   | 0.26        | 0/860         |
| 64  | 3B    | 0.07         | 0/1116  | 0.23        | 0/1490        |
| 65  | 3C    | 0.10         | 0/847   | 0.28        | 0/1135        |
| 66  | 3D    | 0.10         | 0/508   | 0.29        | 0/680         |
| 67  | 3E    | 0.07         | 0/470   | 0.24        | 0/623         |
| 68  | 3F    | 0.08         | 0/2493  | 0.28        | 0/3394        |
| 69  | 3G    | 0.09         | 0/1773  | 0.30        | 0/2395        |
| 70  | 3H    | 0.08         | 0/1946  | 0.24        | 0/2590        |
| 71  | 3I    | 0.10         | 0/1561  | 0.27        | 0/2083        |
| 72  | 3J    | 0.09         | 0/952   | 0.23        | 0/1279        |
| 73  | 3K    | 0.10         | 0/1232  | 0.23        | 0/1656        |
| 74  | 3L    | 0.11         | 0/1062  | 0.31        | 0/1425        |
| 75  | 3M    | 0.09         | 0/1051  | 0.26        | 0/1406        |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 76  | 3N    | 0.10         | 0/1094   | 0.28        | 0/1452          |
| 77  | 3O    | 0.11         | 0/604    | 0.36        | 0/810           |
| 78  | 3P    | 0.09         | 0/665    | 0.27        | 0/891           |
| 79  | 3Q    | 0.14         | 0/465    | 0.26        | 0/612           |
| 80  | 3R    | 0.08         | 0/560    | 0.27        | 0/745           |
| All | All   | 0.10         | 0/232946 | 0.25        | 3/341996 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 61  | 20    | 89  | PRO  | N-CD-CG | -7.51 | 91.94       | 103.20   |
| 61  | 20    | 89  | PRO  | CA-N-CD | -7.00 | 102.21      | 112.00   |
| 20  | 2L    | 78  | ILE  | N-CA-C  | -5.51 | 108.13      | 113.53   |

There are no chirality outliers.

There are no planarity outliers.

## 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   | 1A    | 79674 | 0        | 40254    | 3068    | 0            |
| 2   | 1B    | 2558  | 0        | 1296     | 72      | 0            |
| 3   | 1C    | 3310  | 0        | 1680     | 131     | 0            |
| 4   | 1D    | 1898  | 0        | 1993     | 96      | 0            |
| 5   | 1E    | 3238  | 0        | 3376     | 119     | 0            |
| 6   | 1F    | 2927  | 0        | 3104     | 97      | 0            |
| 7   | 1G    | 2382  | 0        | 2410     | 113     | 0            |
| 8   | 1H    | 1904  | 0        | 2055     | 116     | 0            |
| 9   | 2A    | 1878  | 0        | 2009     | 70      | 0            |
| 10  | 2B    | 1935  | 0        | 2087     | 85      | 0            |
| 11  | 2C    | 1518  | 0        | 1601     | 95      | 0            |
| 12  | 2D    | 1711  | 0        | 1749     | 75      | 0            |
| 13  | 2E    | 1410  | 0        | 1441     | 122     | 0            |
| 14  | 2F    | 1701  | 0        | 1818     | 89      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15  | 2G    | 1138  | 0        | 1204     | 59      | 0            |
| 16  | 2H    | 1701  | 0        | 1749     | 62      | 0            |
| 17  | 2I    | 1650  | 0        | 1794     | 66      | 0            |
| 18  | 2J    | 1242  | 0        | 1269     | 40      | 0            |
| 19  | 2K    | 1513  | 0        | 1628     | 45      | 0            |
| 20  | 2L    | 1566  | 0        | 1729     | 57      | 0            |
| 21  | 2M    | 1453  | 0        | 1490     | 58      | 0            |
| 22  | 2N    | 1298  | 0        | 1366     | 57      | 0            |
| 23  | 2O    | 825   | 0        | 850      | 74      | 0            |
| 24  | 2P    | 979   | 0        | 1039     | 27      | 0            |
| 25  | 2Q    | 1015  | 0        | 1079     | 78      | 0            |
| 26  | 2R    | 985   | 0        | 1066     | 42      | 0            |
| 27  | 2S    | 1115  | 0        | 1205     | 48      | 0            |
| 28  | 2T    | 1107  | 0        | 1182     | 55      | 0            |
| 29  | 2U    | 1162  | 0        | 1213     | 38      | 0            |
| 30  | 2V    | 882   | 0        | 959      | 52      | 0            |
| 31  | 2W    | 764   | 0        | 804      | 43      | 0            |
| 32  | 2X    | 888   | 0        | 930      | 36      | 0            |
| 33  | 2Y    | 1053  | 0        | 1147     | 31      | 0            |
| 34  | 2Z    | 876   | 0        | 912      | 26      | 0            |
| 35  | 2a    | 906   | 0        | 1002     | 51      | 0            |
| 36  | 2b    | 1015  | 0        | 1148     | 43      | 0            |
| 37  | 2c    | 832   | 0        | 917      | 32      | 0            |
| 38  | 2d    | 713   | 0        | 750      | 19      | 0            |
| 39  | 2e    | 569   | 0        | 637      | 36      | 0            |
| 40  | 2f    | 444   | 0        | 483      | 17      | 0            |
| 41  | 2g    | 430   | 0        | 465      | 21      | 0            |
| 42  | 2h    | 230   | 0        | 276      | 9       | 0            |
| 43  | 2i    | 870   | 0        | 946      | 44      | 0            |
| 44  | 2j    | 708   | 0        | 756      | 25      | 0            |
| 45  | 2k    | 1002  | 0        | 1068     | 35      | 0            |
| 46  | 2l    | 1740  | 0        | 1854     | 215     | 0            |
| 47  | 2m    | 36900 | 0        | 18597    | 2048    | 0            |
| 48  | 2n    | 1741  | 0        | 1746     | 201     | 0            |
| 49  | 2o    | 1738  | 0        | 1809     | 137     | 0            |
| 50  | 2p    | 1765  | 0        | 1865     | 252     | 0            |
| 51  | 2q    | 2076  | 0        | 2177     | 171     | 0            |
| 52  | 2r    | 1495  | 0        | 1549     | 218     | 0            |
| 53  | 2s    | 1497  | 0        | 1590     | 174     | 0            |
| 54  | 2t    | 1686  | 0        | 1772     | 142     | 0            |
| 55  | 2u    | 827   | 0        | 854      | 112     | 0            |
| 56  | 2v    | 1247  | 0        | 1323     | 94      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | 2w    | 1045  | 0        | 1095     | 152     | 0            |
| 58  | 2x    | 1124  | 0        | 1193     | 204     | 0            |
| 59  | 2y    | 1090  | 0        | 1149     | 160     | 0            |
| 60  | 2z    | 1198  | 0        | 1261     | 177     | 0            |
| 61  | 20    | 1112  | 0        | 1146     | 135     | 0            |
| 62  | 21    | 817   | 0        | 882      | 105     | 0            |
| 63  | 3A    | 636   | 0        | 637      | 58      | 0            |
| 64  | 3B    | 1098  | 0        | 1167     | 75      | 0            |
| 65  | 3C    | 829   | 0        | 883      | 73      | 0            |
| 66  | 3D    | 506   | 0        | 536      | 75      | 0            |
| 67  | 3E    | 459   | 0        | 450      | 61      | 0            |
| 68  | 3F    | 2436  | 0        | 2393     | 292     | 0            |
| 69  | 3G    | 1733  | 0        | 1826     | 159     | 0            |
| 70  | 3H    | 1923  | 0        | 2089     | 238     | 0            |
| 71  | 3I    | 1533  | 0        | 1653     | 148     | 0            |
| 72  | 3J    | 942   | 0        | 961      | 97      | 0            |
| 73  | 3K    | 1208  | 0        | 1294     | 85      | 0            |
| 74  | 3L    | 1049  | 0        | 1073     | 79      | 0            |
| 75  | 3M    | 1034  | 0        | 1080     | 76      | 0            |
| 76  | 3N    | 1073  | 0        | 1155     | 144     | 0            |
| 77  | 3O    | 598   | 0        | 656      | 151     | 0            |
| 78  | 3P    | 651   | 0        | 672      | 47      | 0            |
| 79  | 3Q    | 459   | 0        | 503      | 34      | 0            |
| 80  | 3R    | 548   | 0        | 555      | 61      | 0            |
| 81  | 1A    | 651   | 777      | 0        | 20      | 0            |
| 81  | 2m    | 93    | 111      | 0        | 6       | 0            |
| 82  | 1A    | 270   | 0        | 0        | 0       | 0            |
| 82  | 1B    | 2     | 0        | 0        | 0       | 0            |
| 82  | 1C    | 5     | 0        | 0        | 0       | 0            |
| 82  | 1D    | 1     | 0        | 0        | 0       | 0            |
| 82  | 20    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2H    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2J    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2K    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2M    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2P    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2V    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2Z    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2a    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2d    | 1     | 0        | 0        | 0       | 0            |
| 82  | 2m    | 105   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 82  | 3H    | 1      | 0        | 0        | 0       | 0            |
| 82  | 3K    | 1      | 0        | 0        | 0       | 0            |
| 82  | 3L    | 1      | 0        | 0        | 0       | 0            |
| 83  | 2d    | 1      | 0        | 0        | 0       | 0            |
| 83  | 2g    | 1      | 0        | 0        | 0       | 0            |
| 83  | 2j    | 1      | 0        | 0        | 0       | 0            |
| 83  | 3C    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 217933 | 888      | 161381   | 10895   | 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 29.

All (10895) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:2x:72:VAL:HG21  | 58:2x:84:ILE:HD11  | 1.20                     | 1.18              |
| 65:3C:44:ILE:HG21  | 65:3C:67:LEU:HD13  | 1.19                     | 1.17              |
| 68:3F:32:LEU:HD21  | 68:3F:71:ILE:HD11  | 1.22                     | 1.15              |
| 77:3O:99:LEU:HD21  | 77:3O:102:LYS:HB3  | 1.19                     | 1.15              |
| 55:2u:25:LYS:HD3   | 55:2u:46:MET:HE1   | 1.18                     | 1.15              |
| 1:1A:5027:C:H2'    | 54:2t:77:ARG:HH22  | 1.13                     | 1.14              |
| 30:2V:23:LYS:HG3   | 30:2V:24:PRO:HD2   | 1.28                     | 1.13              |
| 47:2m:1047:C:H5''  | 74:3L:143:LYS:HB2  | 1.30                     | 1.13              |
| 50:2p:148:LYS:HB2  | 50:2p:150:MET:HE1  | 1.26                     | 1.12              |
| 1:1A:3692:A:H62    | 1:1A:3823:G:N2     | 1.46                     | 1.11              |
| 12:2D:54:SER:HB3   | 12:2D:135:ILE:HD11 | 1.33                     | 1.11              |
| 54:2t:151:GLU:HA   | 54:2t:154:LYS:HE3  | 1.32                     | 1.10              |
| 50:2p:127:MET:HE1  | 50:2p:134:CYS:HB3  | 1.31                     | 1.10              |
| 47:2m:655:A:H4'    | 47:2m:656:G:H5'    | 1.30                     | 1.10              |
| 60:2z:1:MET:HE1    | 77:3O:90:GLU:HB3   | 1.25                     | 1.09              |
| 50:2p:135:GLU:HG3  | 50:2p:153:VAL:HB   | 1.33                     | 1.09              |
| 68:3F:197:THR:HB   | 68:3F:239:LEU:HD12 | 1.31                     | 1.09              |
| 1:1A:3692:A:N6     | 1:1A:3823:G:H21    | 1.47                     | 1.09              |
| 47:2m:1112:U:H2'   | 47:2m:1113:A:H4'   | 1.31                     | 1.09              |
| 53:2s:7:LYS:HE3    | 53:2s:24:SER:HB3   | 1.31                     | 1.09              |
| 50:2p:101:GLN:HG3  | 50:2p:126:ILE:HD11 | 1.34                     | 1.08              |
| 53:2s:144:ILE:HG13 | 53:2s:154:ILE:HG13 | 1.34                     | 1.08              |
| 56:2v:82:MET:HG2   | 56:2v:85:THR:HB    | 1.36                     | 1.07              |
| 60:2z:78:LYS:HD2   | 60:2z:78:LYS:O     | 1.54                     | 1.07              |
| 50:2p:68:GLU:HB2   | 55:2u:20:VAL:HG11  | 1.34                     | 1.07              |
| 58:2x:34:VAL:HG13  | 58:2x:70:VAL:HB    | 1.34                     | 1.07              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:3F:27:PHE:HB2   | 68:3F:30:MET:HE3   | 1.37                     | 1.06              |
| 70:3H:63:MET:HA    | 70:3H:63:MET:HE3   | 1.37                     | 1.05              |
| 55:2u:19:GLY:HA2   | 55:2u:71:LEU:HD12  | 1.35                     | 1.04              |
| 1:1A:1171:G:N2     | 1:1A:1190:C:O2     | 1.89                     | 1.04              |
| 1:1A:2789:A:O2'    | 40:2f:45:ARG:NH2   | 1.91                     | 1.03              |
| 47:2m:150:A:H62    | 47:2m:168:C:N4     | 1.55                     | 1.03              |
| 77:3O:79:ILE:HG21  | 77:3O:84:ALA:HB2   | 1.41                     | 1.03              |
| 47:2m:549:C:O2'    | 47:2m:550:C:O5'    | 1.75                     | 1.03              |
| 54:2t:79:ILE:HD13  | 54:2t:170:LYS:HD3  | 1.41                     | 1.03              |
| 77:3O:47:LEU:HD21  | 77:3O:83:LEU:HB2   | 1.42                     | 1.02              |
| 47:2m:377:G:H5'    | 54:2t:98:LYS:HB3   | 1.37                     | 1.02              |
| 62:21:24:LEU:HD11  | 62:21:87:ARG:HB2   | 1.37                     | 1.02              |
| 68:3F:17:TRP:HB2   | 68:3F:36:ARG:HD3   | 1.42                     | 1.02              |
| 69:3G:74:LYS:HE3   | 69:3G:269:PHE:HB3  | 1.37                     | 1.02              |
| 51:2q:95:THR:HB    | 76:3N:16:ARG:HD3   | 1.34                     | 1.02              |
| 58:2x:97:GLN:HB2   | 58:2x:105:LYS:HD3  | 1.40                     | 1.02              |
| 62:21:38:ASP:HA    | 62:21:41:ARG:HD3   | 1.42                     | 1.01              |
| 60:2z:5:ILE:HD12   | 60:2z:6:PRO:HD2    | 1.40                     | 1.01              |
| 68:3F:77:PHE:HB3   | 68:3F:89:LEU:HD11  | 1.42                     | 1.01              |
| 70:3H:50:VAL:HG21  | 70:3H:111:LEU:HB3  | 1.41                     | 1.01              |
| 72:3J:79:VAL:HG21  | 72:3J:85:LEU:HD22  | 1.40                     | 1.01              |
| 20:2L:183:GLU:HA   | 20:2L:186:LYS:HE3  | 1.36                     | 1.01              |
| 27:2S:82:ILE:HD12  | 27:2S:99:ILE:HD11  | 1.39                     | 1.01              |
| 1:1A:3947:A:H2'    | 1:1A:3948:C:H5''   | 1.43                     | 1.00              |
| 67:3E:11:PRO:HB2   | 67:3E:13:LYS:HG2   | 1.39                     | 1.00              |
| 57:2w:83:MET:HG3   | 57:2w:116:LEU:HD23 | 1.43                     | 1.00              |
| 47:2m:643:A:H4'    | 47:2m:644:G:H5'    | 1.42                     | 1.00              |
| 74:3L:44:VAL:HG12  | 74:3L:53:ILE:HB    | 1.41                     | 1.00              |
| 13:2E:151:ILE:HD11 | 13:2E:156:ARG:HG2  | 1.41                     | 0.99              |
| 66:3D:63:ARG:HG3   | 66:3D:64:GLU:HG3   | 1.40                     | 0.99              |
| 23:2O:19:LEU:HB3   | 23:2O:74:SER:O     | 1.62                     | 0.99              |
| 47:2m:878:G:O6     | 47:2m:908:A:N1     | 1.96                     | 0.99              |
| 1:1A:2465:C:H1'    | 1:1A:3672:G:H22    | 1.24                     | 0.99              |
| 12:2D:180:GLU:HG3  | 12:2D:184:MET:HE1  | 1.42                     | 0.99              |
| 52:2r:143:PRO:HA   | 52:2r:146:ARG:HG2  | 1.44                     | 0.99              |
| 1:1A:1442:C:HO2'   | 1:1A:1443:A:H8     | 1.02                     | 0.98              |
| 51:2q:43:PRO:HG2   | 51:2q:46:ILE:HG12  | 1.45                     | 0.98              |
| 1:1A:1438:U:H3'    | 1:1A:1439:C:H5'    | 1.44                     | 0.98              |
| 1:1A:4233:A:H4'    | 43:2i:98:LYS:HE2   | 1.45                     | 0.98              |
| 47:2m:165:G:H4'    | 70:3H:53:SER:HB2   | 1.43                     | 0.98              |
| 51:2q:208:VAL:HG11 | 51:2q:225:ILE:HG13 | 1.43                     | 0.98              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4896:G:H2'    | 1:1A:4897:G:H8     | 1.26                     | 0.98              |
| 1:1A:4279:A:H5'    | 1:1A:4281:A:H1'    | 1.44                     | 0.97              |
| 58:2x:15:ARG:HG2   | 58:2x:20:THR:HG23  | 1.44                     | 0.97              |
| 47:2m:925:G:H1     | 47:2m:1017:U:H3    | 1.06                     | 0.97              |
| 1:1A:3946:G:H1     | 1:1A:4067:U:H3     | 1.09                     | 0.97              |
| 1:1A:3974:G:H2'    | 1:1A:3975:C:H5'    | 1.46                     | 0.97              |
| 31:2W:37:MET:HA    | 31:2W:37:MET:HE3   | 1.44                     | 0.97              |
| 47:2m:944:A:H1'    | 74:3L:136:PRO:HB3  | 1.47                     | 0.96              |
| 59:2y:24:LEU:HD11  | 59:2y:58:MET:HE2   | 1.46                     | 0.96              |
| 1:1A:452:A:H4'     | 1:1A:453:G:H5'     | 1.44                     | 0.96              |
| 1:1A:4896:G:H2'    | 1:1A:4897:G:C8     | 2.00                     | 0.96              |
| 58:2x:43:GLU:HB3   | 58:2x:44:PRO:HD2   | 1.48                     | 0.96              |
| 1:1A:2694:G:H4'    | 1:1A:2695:A:H5'    | 1.47                     | 0.96              |
| 13:2E:56:THR:HB    | 13:2E:63:ARG:HA    | 1.48                     | 0.96              |
| 47:2m:73:C:H4'     | 47:2m:74:G:H5'     | 1.45                     | 0.96              |
| 1:1A:4993:G:H1     | 1:1A:5058:A:H2     | 1.02                     | 0.96              |
| 1:1A:5023:C:H3'    | 1:1A:5024:C:H4'    | 1.47                     | 0.96              |
| 77:3O:57:LYS:HE2   | 77:3O:77:LEU:HD22  | 1.47                     | 0.96              |
| 47:2m:693:A:H2'    | 47:2m:694:G:H5''   | 1.48                     | 0.95              |
| 47:2m:1547:C:N4    | 47:2m:1586:U:O4    | 1.98                     | 0.95              |
| 1:1A:2669:C:O2'    | 1:1A:2670:C:O5'    | 1.84                     | 0.95              |
| 10:2B:162:ASP:HB3  | 10:2B:163:PRO:HD3  | 1.45                     | 0.95              |
| 14:2F:47:ALA:HB3   | 14:2F:48:PRO:HD3   | 1.47                     | 0.95              |
| 19:2K:39:THR:HG22  | 19:2K:41:SER:H     | 1.30                     | 0.95              |
| 21:2M:164:LYS:HB3  | 21:2M:165:PRO:HD3  | 1.48                     | 0.95              |
| 47:2m:493:A:H1'    | 47:2m:574:A:H5'    | 1.48                     | 0.95              |
| 77:3O:74:SER:HA    | 77:3O:79:ILE:HB    | 1.48                     | 0.95              |
| 19:2K:50:ARG:HA    | 19:2K:53:MET:HG3   | 1.49                     | 0.95              |
| 47:2m:1215:C:H42   | 47:2m:1220:A:H61   | 1.03                     | 0.95              |
| 72:3J:49:LEU:HA    | 72:3J:74:ILE:HG23  | 1.48                     | 0.95              |
| 76:3N:7:ILE:HD12   | 76:3N:27:VAL:HG22  | 1.46                     | 0.95              |
| 47:2m:1748:G:H1    | 47:2m:1786:U:H3    | 1.05                     | 0.95              |
| 67:3E:2:GLY:HA3    | 67:3E:6:LEU:HD11   | 1.47                     | 0.95              |
| 1:1A:2638:G:N2     | 1:1A:2697:A:N1     | 2.15                     | 0.95              |
| 47:2m:338:G:H5'    | 47:2m:339:A:H8     | 1.30                     | 0.94              |
| 37:2c:63:VAL:HG23  | 37:2c:65:LYS:HG3   | 1.49                     | 0.94              |
| 48:2n:145:ILE:HG12 | 48:2n:159:ILE:HD13 | 1.46                     | 0.94              |
| 68:3F:70:VAL:HG11  | 68:3F:112:ALA:HA   | 1.49                     | 0.94              |
| 1:1A:667:A:H5''    | 1:1A:668:C:H5''    | 1.50                     | 0.94              |
| 47:2m:30:C:O2'     | 47:2m:596:U:OP1    | 1.85                     | 0.94              |
| 68:3F:83:TRP:HA    | 68:3F:107:ASP:HB2  | 1.48                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:72:LYS:HD3    | 30:2V:119:CYS:HB3  | 1.50                     | 0.94              |
| 68:3F:164:ILE:HG22 | 68:3F:178:ASN:HA   | 1.49                     | 0.94              |
| 47:2m:731:G:H5''   | 47:2m:732:U:H5''   | 1.48                     | 0.94              |
| 55:2u:90:VAL:HB    | 55:2u:94:LEU:HG    | 1.48                     | 0.94              |
| 47:2m:519:A:H5''   | 71:3I:11:LYS:HE2   | 1.50                     | 0.94              |
| 1:1A:3717:A:H2'    | 1:1A:3718:A:H8     | 1.31                     | 0.94              |
| 1:1A:4137:C:O2     | 1:1A:4147:G:N2     | 1.99                     | 0.93              |
| 36:2b:88:THR:HB    | 36:2b:91:MET:HG3   | 1.50                     | 0.93              |
| 68:3F:87:LEU:HD21  | 68:3F:111:VAL:HG11 | 1.46                     | 0.93              |
| 47:2m:1277:C:O2    | 47:2m:1320:G:N2    | 2.00                     | 0.93              |
| 53:2s:145:ARG:HE   | 75:3M:49:GLU:HG2   | 1.33                     | 0.93              |
| 46:2l:36:ILE:HD11  | 46:2l:165:LEU:HD13 | 1.48                     | 0.93              |
| 68:3F:247:TRP:HB3  | 68:3F:258:ILE:HG23 | 1.51                     | 0.93              |
| 1:1A:2786:C:H5''   | 1:1A:2787:A:H5'    | 1.49                     | 0.93              |
| 72:3J:42:LEU:HD21  | 72:3J:110:VAL:HG21 | 1.49                     | 0.93              |
| 47:2m:337:C:H2'    | 47:2m:338:G:H4'    | 1.50                     | 0.93              |
| 1:1A:3786:U:OP1    | 1:1A:4550:G:O2'    | 1.85                     | 0.93              |
| 56:2v:33:LEU:HD12  | 56:2v:34:PRO:HD2   | 1.49                     | 0.93              |
| 77:3O:79:ILE:CG2   | 77:3O:84:ALA:HB2   | 1.99                     | 0.93              |
| 1:1A:702:U:H2'     | 1:1A:703:G:H4'     | 1.52                     | 0.93              |
| 47:2m:1552:G:H2'   | 50:2p:3:VAL:HG11   | 1.51                     | 0.93              |
| 27:2S:47:MET:HE1   | 27:2S:118:ILE:HG22 | 1.49                     | 0.92              |
| 47:2m:24:C:HO2'    | 47:2m:25:A:H8      | 1.04                     | 0.92              |
| 46:2l:92:LYS:HD3   | 46:2l:97:LYS:HG3   | 1.50                     | 0.92              |
| 47:2m:128:U:OP2    | 47:2m:214:U:O2'    | 1.84                     | 0.92              |
| 64:3B:68:LYS:HB3   | 64:3B:91:LEU:HD22  | 1.47                     | 0.92              |
| 47:2m:150:A:H62    | 47:2m:168:C:H42    | 0.99                     | 0.92              |
| 22:2N:137:GLU:OE1  | 22:2N:137:GLU:N    | 2.03                     | 0.92              |
| 31:2W:20:LEU:HD23  | 31:2W:101:ASP:HB2  | 1.48                     | 0.92              |
| 47:2m:794:A:H2'    | 47:2m:795:A:H4'    | 1.47                     | 0.92              |
| 4:1D:142:GLU:OE1   | 4:1D:142:GLU:N     | 2.02                     | 0.92              |
| 12:2D:76:MET:HE1   | 12:2D:148:VAL:HG12 | 1.51                     | 0.92              |
| 48:2n:159:ILE:HD11 | 63:3A:34:MET:HE1   | 1.51                     | 0.92              |
| 51:2q:42:LEU:HG    | 51:2q:46:ILE:HD11  | 1.51                     | 0.92              |
| 1:1A:963:G:O6      | 1:1A:2095:A:N6     | 2.03                     | 0.92              |
| 46:2l:54:ARG:HG2   | 46:2l:152:LYS:HD2  | 1.51                     | 0.92              |
| 47:2m:957:A:H2'    | 47:2m:958:G:H21    | 1.34                     | 0.92              |
| 50:2p:39:VAL:HG22  | 50:2p:48:ILE:HG12  | 1.50                     | 0.92              |
| 5:1E:317:LEU:HD21  | 5:1E:382:MET:HG2   | 1.52                     | 0.92              |
| 1:1A:1578:U:OP1    | 1:1A:3637:U:O2'    | 1.89                     | 0.91              |
| 59:2y:36:GLU:HB3   | 59:2y:47:ARG:HD2   | 1.52                     | 0.91              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1920:C:H3'    | 1:1A:1921:C:H5''   | 1.52                     | 0.91              |
| 20:2L:178:GLN:HA   | 20:2L:181:LYS:HE3  | 1.52                     | 0.91              |
| 61:20:133:ARG:HH11 | 61:20:134:ILE:HG22 | 1.34                     | 0.91              |
| 77:3O:47:LEU:HD22  | 77:3O:79:ILE:HD12  | 1.53                     | 0.91              |
| 1:1A:2299:G:O2'    | 1:1A:2300:A:OP1    | 1.87                     | 0.91              |
| 47:2m:215:G:O2'    | 47:2m:216:C:O2     | 1.88                     | 0.91              |
| 57:2w:81:ARG:HA    | 57:2w:116:LEU:HD11 | 1.50                     | 0.91              |
| 75:3M:28:ARG:HB3   | 75:3M:29:PRO:HD3   | 1.52                     | 0.91              |
| 13:2E:96:LYS:HG2   | 13:2E:163:MET:HE1  | 1.52                     | 0.91              |
| 60:2z:13:LEU:HD23  | 60:2z:20:ILE:HD11  | 1.52                     | 0.91              |
| 16:2H:124:ASP:OD1  | 16:2H:125:SER:N    | 2.03                     | 0.91              |
| 45:2k:26:SER:OG    | 45:2k:28:GLU:OE2   | 1.88                     | 0.91              |
| 76:3N:6:THR:HG22   | 76:3N:28:LEU:HB2   | 1.51                     | 0.91              |
| 54:2t:141:ARG:HB3  | 54:2t:145:ILE:HD11 | 1.53                     | 0.90              |
| 1:1A:2705:G:N1     | 1:1A:2710:C:N3     | 2.18                     | 0.90              |
| 47:2m:1511:U:O2'   | 47:2m:1512:C:H5'   | 1.70                     | 0.90              |
| 1:1A:2907:G:H1'    | 1:1A:3589:G:H1     | 1.35                     | 0.90              |
| 1:1A:4099:G:O2'    | 1:1A:4100:C:O4'    | 1.88                     | 0.90              |
| 25:2Q:105:ARG:HH12 | 70:3H:151:ASP:HA   | 1.36                     | 0.90              |
| 46:2l:179:LEU:HA   | 46:2l:182:ASN:HB3  | 1.53                     | 0.90              |
| 47:2m:1446:A:H1'   | 62:21:55:ARG:HD2   | 1.51                     | 0.90              |
| 1:1A:1187:G:OP2    | 1:1A:1187:G:N2     | 2.03                     | 0.90              |
| 62:21:35:VAL:HG21  | 62:21:107:GLU:HG2  | 1.52                     | 0.90              |
| 14:2F:211:LYS:HE2  | 46:2l:184:HIS:HB2  | 1.52                     | 0.90              |
| 1:1A:2806:A:H1'    | 35:2a:4:ARG:HD3    | 1.53                     | 0.90              |
| 65:3C:44:ILE:CG2   | 65:3C:67:LEU:HD13  | 2.01                     | 0.90              |
| 25:2Q:97:LYS:HG2   | 25:2Q:98:PRO:HD3   | 1.51                     | 0.90              |
| 52:2r:134:VAL:HG12 | 52:2r:135:ARG:HG2  | 1.54                     | 0.90              |
| 47:2m:150:A:N6     | 47:2m:168:C:H42    | 1.69                     | 0.89              |
| 1:1A:3945:A:H2'    | 1:1A:3946:G:H5''   | 1.54                     | 0.89              |
| 1:1A:3974:G:H1     | 1:1A:4050:A:H2'    | 1.36                     | 0.89              |
| 50:2p:106:ARG:HG3  | 50:2p:175:VAL:HG22 | 1.54                     | 0.89              |
| 11:2C:118:LEU:HD11 | 11:2C:167:VAL:HG22 | 1.54                     | 0.89              |
| 49:2o:196:ASP:HA   | 49:2o:199:LYS:NZ   | 1.86                     | 0.89              |
| 1:1A:2765:A:H2'    | 1:1A:2766:A:H5'    | 1.55                     | 0.89              |
| 1:1A:3717:A:H2'    | 1:1A:3718:A:C8     | 2.06                     | 0.89              |
| 47:2m:1421:A:H2'   | 61:20:2:PRO:HB2    | 1.55                     | 0.89              |
| 47:2m:981:A:H2'    | 47:2m:982:G:C8     | 2.08                     | 0.89              |
| 71:3I:122:SER:O    | 71:3I:125:HIS:N    | 2.07                     | 0.88              |
| 60:2z:5:ILE:HD13   | 77:3O:49:LEU:HB3   | 1.54                     | 0.88              |
| 1:1A:4883:C:H4'    | 1:1A:4884:G:H5'    | 1.54                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:2C:18:ILE:HG22  | 11:2C:27:VAL:HG22  | 1.55                     | 0.88              |
| 1:1A:2101:C:H2'    | 1:1A:2102:G:N7     | 1.88                     | 0.88              |
| 52:2r:76:MET:HE1   | 52:2r:169:ILE:HD11 | 1.53                     | 0.88              |
| 47:2m:750:C:H42    | 47:2m:794:A:H1'    | 1.38                     | 0.88              |
| 13:2E:12:MET:HA    | 13:2E:12:MET:HE3   | 1.54                     | 0.88              |
| 47:2m:1517:G:O2'   | 47:2m:1518:C:O4'   | 1.92                     | 0.88              |
| 47:2m:1542:C:H4'   | 61:20:11:GLN:HB3   | 1.52                     | 0.88              |
| 50:2p:55:THR:HA    | 50:2p:58:VAL:HG12  | 1.55                     | 0.88              |
| 54:2t:105:ASP:OD1  | 54:2t:107:THR:HG23 | 1.73                     | 0.88              |
| 70:3H:195:LYS:HG3  | 70:3H:198:ARG:HH21 | 1.36                     | 0.88              |
| 1:1A:2903:G:H4'    | 1:1A:3591:C:H42    | 1.37                     | 0.88              |
| 1:1A:3599:A:H2'    | 1:1A:3600:G:H8     | 1.38                     | 0.88              |
| 1:1A:3616:U:H4'    | 1:1A:3617:G:H5'    | 1.56                     | 0.88              |
| 46:2l:24:LYS:HE2   | 46:2l:29:LEU:HD13  | 1.56                     | 0.88              |
| 47:2m:1314:U:O2'   | 55:2u:1:MET:O      | 1.92                     | 0.88              |
| 61:20:5:THR:HG23   | 61:20:7:LYS:H      | 1.39                     | 0.88              |
| 1:1A:3951:G:N2     | 1:1A:4061:G:O6     | 2.06                     | 0.88              |
| 47:2m:1119:A:O2'   | 47:2m:1120:U:O4'   | 1.92                     | 0.88              |
| 1:1A:4103:C:O2'    | 1:1A:4106:G:N2     | 2.07                     | 0.87              |
| 46:2l:120:ILE:HG23 | 46:2l:124:LEU:HD13 | 1.53                     | 0.87              |
| 47:2m:1060:A:O2'   | 47:2m:1062:A:N7    | 2.07                     | 0.87              |
| 47:2m:942:G:H21    | 74:3L:137:SER:HB2  | 1.39                     | 0.87              |
| 58:2x:39:LEU:HD12  | 58:2x:51:LEU:HD21  | 1.56                     | 0.87              |
| 1:1A:2705:G:H1'    | 1:1A:2712:G:N2     | 1.89                     | 0.87              |
| 74:3L:103:ASN:ND2  | 74:3L:140:THR:O    | 2.08                     | 0.87              |
| 1:1A:1171:G:N1     | 1:1A:1190:C:N3     | 2.23                     | 0.87              |
| 1:1A:3961:G:N2     | 1:1A:4046:A:OP1    | 2.06                     | 0.87              |
| 47:2m:1507:G:H1    | 80:3R:90:LYS:HA    | 1.39                     | 0.87              |
| 72:3J:86:GLY:HA3   | 72:3J:105:GLY:HA2  | 1.55                     | 0.87              |
| 22:2N:115:LYS:HD2  | 22:2N:126:VAL:HG11 | 1.56                     | 0.87              |
| 47:2m:1130:G:H2'   | 47:2m:1131:G:H5''  | 1.54                     | 0.87              |
| 68:3F:297:THR:HG22 | 68:3F:311:GLN:HG2  | 1.55                     | 0.87              |
| 1:1A:4137:C:N3     | 1:1A:4147:G:N1     | 2.22                     | 0.87              |
| 18:2J:94:MET:HG2   | 18:2J:148:MET:HE3  | 1.55                     | 0.87              |
| 1:1A:1200:G:H2'    | 1:1A:1201:U:H5'    | 1.57                     | 0.87              |
| 49:2o:49:VAL:HG11  | 49:2o:62:LEU:HD23  | 1.57                     | 0.87              |
| 52:2r:100:ILE:HD12 | 52:2r:178:ILE:HG23 | 1.57                     | 0.87              |
| 64:3B:32:LEU:HD21  | 64:3B:34:THR:HG22  | 1.57                     | 0.87              |
| 1:1A:128:C:H2'     | 1:1A:129:C:C6      | 2.10                     | 0.87              |
| 1:1A:1763:C:H2'    | 1:1A:1764:G:H5'    | 1.56                     | 0.87              |
| 47:2m:1203:G:H21   | 47:2m:1699:A:H8    | 1.21                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:3J:31:LEU:HA    | 72:3J:112:LYS:HE2  | 1.53                     | 0.87              |
| 1:1A:4988:U:O2'    | 1:1A:4989:U:OP2    | 1.91                     | 0.87              |
| 25:2Q:101:ARG:HB2  | 25:2Q:105:ARG:HE   | 1.36                     | 0.87              |
| 47:2m:1752:C:H2'   | 47:2m:1753:C:H5'   | 1.57                     | 0.87              |
| 68:3F:173:LEU:HG   | 68:3F:189:ILE:HG23 | 1.57                     | 0.87              |
| 46:2l:54:ARG:HG3   | 46:2l:154:THR:HB   | 1.57                     | 0.86              |
| 47:2m:732:U:OP1    | 47:2m:733:C:N4     | 2.07                     | 0.86              |
| 51:2q:246:LEU:HB3  | 51:2q:250:GLU:HG3  | 1.55                     | 0.86              |
| 1:1A:2856:C:O2     | 5:1E:242:ARG:NH2   | 2.08                     | 0.86              |
| 35:2a:107:LEU:HD12 | 35:2a:110:GLN:HE21 | 1.39                     | 0.86              |
| 46:2l:105:LYS:NZ   | 46:2l:127:GLY:O    | 2.08                     | 0.86              |
| 47:2m:1144:A:H5'   | 47:2m:1355:C:H41   | 1.37                     | 0.86              |
| 1:1A:319:A:H1'     | 1:1A:3726:A:H8     | 1.37                     | 0.86              |
| 1:1A:2659:A:N6     | 1:1A:2675:G:H1'    | 1.90                     | 0.86              |
| 5:1E:153:MET:HG3   | 5:1E:194:LEU:HD11  | 1.57                     | 0.86              |
| 53:2s:101:LEU:HD23 | 53:2s:102:PRO:HD2  | 1.57                     | 0.86              |
| 31:2W:38:ILE:HD11  | 31:2W:46:VAL:HG21  | 1.58                     | 0.86              |
| 47:2m:1264:C:H4'   | 47:2m:1265:A:H5'   | 1.57                     | 0.86              |
| 51:2q:60:GLU:O     | 51:2q:64:ILE:HG23  | 1.74                     | 0.86              |
| 64:3B:87:ASN:ND2   | 64:3B:90:CYS:SG    | 2.49                     | 0.86              |
| 7:1G:41:LYS:HE2    | 22:2N:93:ILE:HD13  | 1.56                     | 0.86              |
| 8:1H:133:PHE:O     | 8:1H:138:ARG:NH2   | 2.09                     | 0.86              |
| 79:3Q:29:THR:HA    | 79:3Q:33:LYS:HD3   | 1.58                     | 0.86              |
| 1:1A:137:G:H2'     | 1:1A:138:G:C8      | 2.11                     | 0.86              |
| 39:2e:49:ASP:HB3   | 39:2e:52:LYS:HG3   | 1.57                     | 0.86              |
| 53:2s:53:VAL:HG23  | 53:2s:175:GLY:HA3  | 1.58                     | 0.86              |
| 77:3O:47:LEU:HD23  | 77:3O:80:ARG:H     | 1.39                     | 0.86              |
| 80:3R:121:CYS:HA   | 80:3R:132:MET:HE3  | 1.55                     | 0.86              |
| 23:2O:19:LEU:HB2   | 23:2O:73:THR:HG23  | 1.58                     | 0.86              |
| 46:2l:54:ARG:HA    | 46:2l:154:THR:HG21 | 1.57                     | 0.86              |
| 49:2o:134:LEU:HG   | 49:2o:218:LEU:HD12 | 1.56                     | 0.86              |
| 76:3N:21:LYS:HB2   | 76:3N:75:ILE:HG22  | 1.57                     | 0.86              |
| 47:2m:1277:C:N3    | 47:2m:1320:G:N1    | 2.22                     | 0.85              |
| 52:2r:168:THR:N    | 52:2r:171:GLU:OE1  | 2.09                     | 0.85              |
| 12:2D:146:GLU:OE1  | 12:2D:146:GLU:N    | 2.07                     | 0.85              |
| 13:2E:120:ASP:HB2  | 13:2E:123:ILE:HG13 | 1.58                     | 0.85              |
| 39:2e:26:LYS:HB2   | 39:2e:69:LEU:HD12  | 1.56                     | 0.85              |
| 1:1A:759:G:H2'     | 1:1A:760:G:H5'     | 1.58                     | 0.85              |
| 1:1A:1078:A:H2'    | 1:1A:1079:C:H5'    | 1.57                     | 0.85              |
| 48:2n:115:ALA:HB1  | 48:2n:117:ARG:HH22 | 1.41                     | 0.85              |
| 53:2s:98:ARG:HB3   | 53:2s:125:VAL:HG22 | 1.56                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 68:3F:258:ILE:HD12 | 68:3F:268:ASP:HB2 | 1.58                     | 0.85              |
| 71:3I:94:LEU:HD12  | 71:3I:97:ILE:HD13 | 1.58                     | 0.85              |
| 53:2s:22:GLY:HA2   | 53:2s:25:GLN:HB2  | 1.58                     | 0.85              |
| 8:1H:223:ARG:HG2   | 8:1H:237:LYS:HD2  | 1.55                     | 0.85              |
| 26:2R:64:SER:HB2   | 36:2b:69:LEU:HD13 | 1.58                     | 0.85              |
| 50:2p:177:LEU:HD23 | 50:2p:178:ARG:HG3 | 1.59                     | 0.85              |
| 1:1A:2760:G:H1'    | 1:1A:2761:U:OP2   | 1.77                     | 0.85              |
| 1:1A:4043:G:OP1    | 1:1A:4045:G:N2    | 2.09                     | 0.85              |
| 65:3C:46:GLU:OE2   | 74:3L:113:GLN:HB3 | 1.76                     | 0.85              |
| 1:1A:418:A:N6      | 3:1C:16:G:H1'     | 1.90                     | 0.85              |
| 47:2m:189:U:H1'    | 47:2m:211:G:H22   | 1.40                     | 0.85              |
| 47:2m:983:A:H2     | 74:3L:139:SER:HB3 | 1.37                     | 0.85              |
| 1:1A:493:G:H2'     | 1:1A:494:U:H5'    | 1.59                     | 0.85              |
| 1:1A:2695:A:H5''   | 39:2e:26:LYS:HE3  | 1.59                     | 0.85              |
| 1:1A:3765:G:H2'    | 1:1A:3766:A:H5'   | 1.59                     | 0.85              |
| 50:2p:132:LYS:HE3  | 50:2p:191:PRO:HA  | 1.57                     | 0.85              |
| 25:2Q:105:ARG:NH1  | 70:3H:151:ASP:HA  | 1.91                     | 0.85              |
| 47:2m:1242:U:O2    | 47:2m:1517:G:H4'  | 1.75                     | 0.85              |
| 57:2w:44:ARG:NH1   | 57:2w:82:ASP:OD1  | 2.10                     | 0.85              |
| 1:1A:1762:C:H3'    | 1:1A:1763:C:H5''  | 1.59                     | 0.84              |
| 1:1A:4734:A:H2'    | 1:1A:4735:G:H8    | 1.39                     | 0.84              |
| 74:3L:61:LYS:NZ    | 74:3L:80:ASP:OD2  | 2.09                     | 0.84              |
| 9:2A:105:VAL:HG13  | 9:2A:136:VAL:HG12 | 1.58                     | 0.84              |
| 27:2S:52:ASP:HB2   | 27:2S:110:LYS:HG3 | 1.59                     | 0.84              |
| 47:2m:669:A:H3'    | 47:2m:669:A:OP2   | 1.76                     | 0.84              |
| 47:2m:1298:G:N7    | 47:2m:1514:G:H1'  | 1.92                     | 0.84              |
| 53:2s:15:LYS:H     | 53:2s:16:PRO:CD   | 1.90                     | 0.84              |
| 1:1A:4620:U:OP2    | 1:1A:4670:C:N4    | 2.10                     | 0.84              |
| 5:1E:107:ALA:HB2   | 5:1E:201:LEU:HG   | 1.60                     | 0.84              |
| 6:1F:290:SER:O     | 6:1F:294:LYS:HG2  | 1.77                     | 0.84              |
| 47:2m:558:G:H2'    | 47:2m:559:G:N2    | 1.92                     | 0.84              |
| 47:2m:878:G:H5'    | 47:2m:879:C:H5    | 1.42                     | 0.84              |
| 69:3G:125:LYS:HG3  | 69:3G:143:CYS:HB2 | 1.57                     | 0.84              |
| 1:1A:2489:C:O2'    | 1:1A:2491:C:N4    | 2.10                     | 0.84              |
| 77:3O:69:THR:HG23  | 77:3O:72:VAL:HG12 | 1.59                     | 0.84              |
| 1:1A:2005:G:H2'    | 1:1A:2006:U:H5    | 1.41                     | 0.84              |
| 47:2m:1518:C:H5''  | 47:2m:1519:U:H5'' | 1.60                     | 0.84              |
| 50:2p:69:LEU:HD22  | 50:2p:86:LEU:HD11 | 1.60                     | 0.84              |
| 1:1A:1763:C:N4     | 1:1A:1770:A:N1    | 2.25                     | 0.84              |
| 47:2m:910:G:H2'    | 47:2m:911:C:O4'   | 1.78                     | 0.84              |
| 47:2m:1488:C:O2'   | 47:2m:1490:G:OP2  | 1.96                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:3A:23:ILE:HD13  | 69:3G:251:LEU:HB2  | 1.58                     | 0.84              |
| 70:3H:30:LYS:HD3   | 70:3H:36:VAL:HG21  | 1.58                     | 0.84              |
| 1:1A:2695:A:H4'    | 1:1A:2696:A:O5'    | 1.78                     | 0.84              |
| 8:1H:281:ILE:HB    | 8:1H:286:LEU:HD21  | 1.59                     | 0.84              |
| 47:2m:1253:A:OP2   | 47:2m:1526:G:N2    | 2.09                     | 0.84              |
| 58:2x:21:ALA:HB2   | 58:2x:72:VAL:HG13  | 1.57                     | 0.84              |
| 60:2z:86:ARG:NH1   | 60:2z:110:ASP:OD2  | 2.11                     | 0.84              |
| 68:3F:163:PRO:HB2  | 68:3F:179:LEU:HD13 | 1.56                     | 0.84              |
| 62:21:56:MET:SD    | 62:21:57:PRO:HD2   | 2.17                     | 0.84              |
| 70:3H:42:GLY:HA3   | 70:3H:45:TRP:HE3   | 1.42                     | 0.84              |
| 1:1A:3960:A:N6     | 1:1A:4045:G:O2'    | 2.11                     | 0.83              |
| 63:3A:42:VAL:HG23  | 63:3A:43:THR:HG23  | 1.58                     | 0.83              |
| 1:1A:265:C:O2'     | 1:1A:266:C:OP2     | 1.96                     | 0.83              |
| 1:1A:4551:U:OP1    | 81:1A:5110:84D:N4  | 2.11                     | 0.83              |
| 46:2l:67:VAL:HG12  | 46:2l:111:LEU:HB2  | 1.59                     | 0.83              |
| 63:3A:80:SER:O     | 63:3A:81:LYS:HG2   | 1.77                     | 0.83              |
| 47:2m:1215:C:N4    | 47:2m:1220:A:H61   | 1.77                     | 0.83              |
| 48:2n:58:LEU:HD12  | 48:2n:161:ILE:HD13 | 1.60                     | 0.83              |
| 48:2n:5:LEU:O      | 48:2n:9:GLN:NE2    | 2.10                     | 0.83              |
| 50:2p:76:ARG:HG3   | 55:2u:22:VAL:HG11  | 1.59                     | 0.83              |
| 25:2Q:14:TYR:HB3   | 25:2Q:15:PRO:HD2   | 1.61                     | 0.83              |
| 69:3G:64:THR:OG1   | 69:3G:90:GLU:OE2   | 1.97                     | 0.83              |
| 77:3O:101:SER:O    | 77:3O:102:LYS:HD3  | 1.77                     | 0.83              |
| 1:1A:935:A:O2'     | 15:2G:44:GLN:O     | 1.96                     | 0.83              |
| 1:1A:2659:A:H61    | 1:1A:2675:G:H1'    | 1.42                     | 0.83              |
| 1:1A:4734:A:H2'    | 1:1A:4735:G:C8     | 2.13                     | 0.83              |
| 47:2m:1414:A:O2'   | 47:2m:1416:C:O3'   | 1.97                     | 0.83              |
| 13:2E:55:TYR:HA    | 13:2E:64:ARG:HB2   | 1.60                     | 0.83              |
| 31:2W:11:LEU:HA    | 31:2W:14:ILE:HG22  | 1.59                     | 0.83              |
| 37:2c:55:ARG:O     | 37:2c:59:GLU:HG2   | 1.79                     | 0.83              |
| 47:2m:125:C:H5''   | 47:2m:126:G:OP1    | 1.79                     | 0.83              |
| 1:1A:1563:A:H2'    | 1:1A:1564:A:C8     | 2.13                     | 0.83              |
| 27:2S:37:GLU:N     | 27:2S:37:GLU:OE1   | 2.11                     | 0.83              |
| 46:2l:103:LEU:HD23 | 46:2l:106:LYS:HA   | 1.59                     | 0.83              |
| 47:2m:1597:C:OP2   | 77:3O:85:ARG:NH2   | 2.12                     | 0.83              |
| 6:1F:298:ILE:O     | 6:1F:302:LEU:HG    | 1.78                     | 0.83              |
| 47:2m:655:A:H4'    | 47:2m:656:G:C5'    | 2.09                     | 0.83              |
| 47:2m:746:C:OP1    | 47:2m:796:G:N2     | 2.11                     | 0.83              |
| 75:3M:87:GLU:N     | 75:3M:87:GLU:OE1   | 2.10                     | 0.83              |
| 47:2m:1560:U:O2    | 47:2m:1575:G:O6    | 1.97                     | 0.83              |
| 52:2r:127:ARG:CG   | 52:2r:137:GLN:HB2  | 2.08                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1273:G:O2'    | 1:1A:1274:A:H5'    | 1.79                     | 0.82              |
| 30:2V:122:LYS:O    | 30:2V:122:LYS:NZ   | 2.11                     | 0.82              |
| 32:2X:59:THR:HB    | 32:2X:60:PRO:HD2   | 1.61                     | 0.82              |
| 47:2m:1452:A:H61   | 47:2m:1474:A:H2'   | 1.43                     | 0.82              |
| 47:2m:1610:G:H2'   | 47:2m:1611:G:C8    | 2.14                     | 0.82              |
| 1:1A:1732:C:O2'    | 1:1A:1733:G:H5'    | 1.78                     | 0.82              |
| 1:1A:4274:A:H2'    | 1:1A:4275:G:H8     | 1.44                     | 0.82              |
| 46:2l:48:ARG:HD3   | 46:2l:49:PHE:H     | 1.43                     | 0.82              |
| 46:2l:93:LEU:O     | 46:2l:102:LYS:NZ   | 2.11                     | 0.82              |
| 47:2m:549:C:H2'    | 47:2m:550:C:C6     | 2.14                     | 0.82              |
| 58:2x:72:VAL:CG2   | 58:2x:84:ILE:HD11  | 2.06                     | 0.82              |
| 65:3C:47:ALA:HA    | 65:3C:50:VAL:CG2   | 2.10                     | 0.82              |
| 75:3M:53:ILE:HD13  | 78:3P:24:LEU:HG    | 1.61                     | 0.82              |
| 1:1A:4874:A:C2     | 17:2l:179:LYS:HG3  | 2.14                     | 0.82              |
| 47:2m:114:G:O2'    | 47:2m:382:C:O2'    | 1.96                     | 0.82              |
| 47:2m:301:A:N3     | 54:2t:73:THR:HG21  | 1.94                     | 0.82              |
| 47:2m:1453:C:H4'   | 59:2y:49:LYS:HA    | 1.61                     | 0.82              |
| 47:2m:1753:C:O2'   | 47:2m:1755:C:N4    | 2.12                     | 0.82              |
| 54:2t:172:LEU:HD11 | 54:2t:195:LEU:HD13 | 1.60                     | 0.82              |
| 1:1A:2484:A:N6     | 1:1A:2495:U:O2     | 2.12                     | 0.82              |
| 47:2m:656:G:H21    | 47:2m:663:C:H5''   | 1.41                     | 0.82              |
| 76:3N:21:LYS:HB2   | 76:3N:75:ILE:CG2   | 2.09                     | 0.82              |
| 59:2y:78:ARG:HG2   | 59:2y:81:ARG:HH21  | 1.43                     | 0.82              |
| 68:3F:247:TRP:HB3  | 68:3F:258:ILE:CG2  | 2.09                     | 0.82              |
| 1:1A:2758:G:O2'    | 1:1A:2764:A:N3     | 2.12                     | 0.82              |
| 7:1G:182:GLY:HA2   | 7:1G:194:VAL:HG22  | 1.60                     | 0.82              |
| 7:1G:234:ASP:O     | 7:1G:235:MET:HG3   | 1.78                     | 0.82              |
| 41:2g:78:ILE:HG23  | 41:2g:83:ARG:HH12  | 1.44                     | 0.82              |
| 47:2m:1776:G:H2'   | 47:2m:1777:G:C8    | 2.15                     | 0.82              |
| 50:2p:23:GLU:OE2   | 55:2u:63:ALA:HB1   | 1.80                     | 0.82              |
| 60:2z:30:ILE:HG12  | 60:2z:71:MET:HE1   | 1.61                     | 0.82              |
| 66:3D:21:THR:HG23  | 66:3D:27:CYS:HB2   | 1.60                     | 0.82              |
| 67:3E:19:ARG:HE    | 67:3E:32:ARG:HD3   | 1.44                     | 0.82              |
| 77:3O:74:SER:HA    | 77:3O:79:ILE:CB    | 2.09                     | 0.82              |
| 1:1A:1202:C:H3'    | 1:1A:1203:G:H5''   | 1.62                     | 0.82              |
| 1:1A:1577:G:O2'    | 1:1A:1612:G:H4'    | 1.78                     | 0.82              |
| 1:1A:1952:G:H4'    | 21:2M:93:MET:HG2   | 1.60                     | 0.82              |
| 1:1A:4594:U:H2'    | 1:1A:4595:G:H8     | 1.44                     | 0.82              |
| 2:1B:120:U:H2'     | 7:1G:258:LYS:HE2   | 1.62                     | 0.82              |
| 65:3C:44:ILE:HD13  | 65:3C:67:LEU:CD1   | 2.09                     | 0.82              |
| 1:1A:4274:A:H2'    | 1:1A:4275:G:C8     | 2.15                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:2B:120:LYS:C    | 10:2B:125:LYS:HG2  | 2.05                     | 0.82              |
| 46:2l:198:TRP:HZ2  | 46:2l:202:ARG:HB2  | 1.44                     | 0.82              |
| 47:2m:835:C:H2'    | 47:2m:837:A:H1'    | 1.62                     | 0.82              |
| 48:2n:85:ARG:HH21  | 48:2n:201:LEU:HD12 | 1.42                     | 0.82              |
| 52:2r:180:ALA:HA   | 52:2r:190:ILE:HD11 | 1.61                     | 0.82              |
| 69:3G:203:GLY:N    | 69:3G:221:ASP:OD1  | 2.13                     | 0.82              |
| 72:3J:68:LEU:HA    | 80:3R:114:ILE:HD11 | 1.59                     | 0.82              |
| 1:1A:3953:G:N2     | 1:1A:4060:U:O4'    | 2.12                     | 0.82              |
| 46:2l:85:MET:SD    | 46:2l:89:ALA:HB3   | 2.19                     | 0.82              |
| 50:2p:76:ARG:HE    | 50:2p:77:PHE:HD1   | 1.24                     | 0.82              |
| 51:2q:102:ILE:HD12 | 51:2q:239:PRO:HD3  | 1.61                     | 0.82              |
| 58:2x:31:LEU:O     | 58:2x:68:ILE:N     | 2.10                     | 0.82              |
| 62:21:26:SER:HB2   | 62:21:110:VAL:HG22 | 1.62                     | 0.82              |
| 2:1B:117:G:OP1     | 7:1G:253:TYR:OH    | 1.98                     | 0.82              |
| 47:2m:507:G:OP1    | 76:3N:108:LYS:NZ   | 2.13                     | 0.82              |
| 47:2m:1348:G:H22   | 47:2m:1381:G:H1    | 1.28                     | 0.82              |
| 13:2E:96:LYS:HB2   | 13:2E:177:GLY:HA3  | 1.60                     | 0.81              |
| 27:2S:4:ASN:HB3    | 27:2S:7:VAL:HG22   | 1.60                     | 0.81              |
| 47:2m:141:A:H4'    | 47:2m:142:C:H5''   | 1.61                     | 0.81              |
| 68:3F:177:TRP:CD1  | 68:3F:184:LEU:HA   | 2.15                     | 0.81              |
| 1:1A:4767:C:O2'    | 1:1A:4874:A:N6     | 2.12                     | 0.81              |
| 6:1F:171:LEU:HD11  | 6:1F:177:TRP:HE3   | 1.42                     | 0.81              |
| 47:2m:1263:U:H4'   | 67:3E:27:ARG:HE    | 1.44                     | 0.81              |
| 52:2r:50:PRO:HG2   | 52:2r:90:VAL:HG13  | 1.61                     | 0.81              |
| 69:3G:135:GLY:HA2  | 69:3G:165:VAL:HB   | 1.62                     | 0.81              |
| 1:1A:2395:A:N3     | 1:1A:2806:A:O2'    | 2.13                     | 0.81              |
| 37:2c:58:MET:HE2   | 37:2c:90:LEU:HD22  | 1.62                     | 0.81              |
| 47:2m:928:G:H1     | 47:2m:1013:U:H3    | 1.28                     | 0.81              |
| 48:2n:66:VAL:HG21  | 48:2n:185:MET:HB2  | 1.63                     | 0.81              |
| 77:3O:58:LEU:HA    | 77:3O:62:VAL:HG11  | 1.62                     | 0.81              |
| 1:1A:1242:G:N3     | 30:2V:120:ARG:NH2  | 2.29                     | 0.81              |
| 12:2D:101:LYS:HE3  | 12:2D:103:LEU:HD13 | 1.63                     | 0.81              |
| 47:2m:1164:G:O2'   | 47:2m:1165:G:H5'   | 1.80                     | 0.81              |
| 53:2s:163:GLN:O    | 53:2s:167:GLU:CB   | 2.29                     | 0.81              |
| 66:3D:24:GLN:OE1   | 66:3D:24:GLN:N     | 2.12                     | 0.81              |
| 72:3J:35:ILE:HA    | 72:3J:38:ALA:HB3   | 1.60                     | 0.81              |
| 1:1A:5027:C:H2'    | 54:2t:77:ARG:NH2   | 1.93                     | 0.81              |
| 25:2Q:101:ARG:HH11 | 25:2Q:105:ARG:HH21 | 1.27                     | 0.81              |
| 51:2q:57:THR:O     | 51:2q:61:VAL:HG23  | 1.81                     | 0.81              |
| 69:3G:105:GLU:OE1  | 69:3G:105:GLU:N    | 2.13                     | 0.81              |
| 25:2Q:80:ARG:HH22  | 70:3H:129:VAL:HG23 | 1.46                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:2i:12:CYS:SG    | 43:2i:14:LYS:NZ    | 2.52                     | 0.81              |
| 47:2m:216:C:N4     | 47:2m:309:G:O6     | 2.13                     | 0.81              |
| 47:2m:1378:A:H4'   | 47:2m:1379:A:O5'   | 1.81                     | 0.81              |
| 47:2m:1454:A:OP2   | 59:2y:3:ARG:NH1    | 2.13                     | 0.81              |
| 76:3N:51:THR:OG1   | 76:3N:53:ASP:OD1   | 1.99                     | 0.81              |
| 1:1A:4625:C:O2'    | 1:1A:4626:A:H5'    | 1.79                     | 0.81              |
| 1:1A:4750:G:H3'    | 1:1A:4751:G:H21    | 1.46                     | 0.81              |
| 80:3R:119:ARG:HB3  | 80:3R:132:MET:HG3  | 1.62                     | 0.81              |
| 1:1A:2705:G:N2     | 1:1A:2710:C:O2     | 2.13                     | 0.81              |
| 1:1A:4768:G:H5'    | 17:2I:176:ARG:HD3  | 1.63                     | 0.81              |
| 1:1A:4964:C:O2'    | 1:1A:4965:U:H5'    | 1.81                     | 0.81              |
| 11:2C:120:GLU:OE2  | 11:2C:124:ARG:NH1  | 2.14                     | 0.81              |
| 47:2m:655:A:C4'    | 47:2m:656:G:H5'    | 2.10                     | 0.81              |
| 1:1A:4869:U:O2'    | 1:1A:4873:G:OP1    | 1.99                     | 0.81              |
| 1:1A:4985:U:O2     | 5:1E:174:ARG:NH1   | 2.14                     | 0.81              |
| 47:2m:207:G:O2'    | 47:2m:208:G:OP1    | 1.97                     | 0.81              |
| 50:2p:137:VAL:HG22 | 50:2p:185:LYS:HB2  | 1.63                     | 0.81              |
| 10:2B:210:GLU:N    | 10:2B:210:GLU:OE1  | 2.14                     | 0.81              |
| 46:2I:66:CYS:HB3   | 46:2I:82:ILE:HD13  | 1.63                     | 0.81              |
| 22:2N:115:LYS:HD3  | 22:2N:126:VAL:HG21 | 1.63                     | 0.80              |
| 47:2m:1447:G:O5'   | 62:2I:87:ARG:NH2   | 2.13                     | 0.80              |
| 52:2r:172:CYS:O    | 52:2r:176:GLU:HG2  | 1.81                     | 0.80              |
| 66:3D:20:ARG:HH21  | 66:3D:26:GLN:HA    | 1.46                     | 0.80              |
| 70:3H:216:ARG:O    | 70:3H:217:MET:HG3  | 1.80                     | 0.80              |
| 77:3O:47:LEU:HB2   | 77:3O:79:ILE:HA    | 1.63                     | 0.80              |
| 77:3O:58:LEU:HD23  | 77:3O:62:VAL:HG11  | 1.61                     | 0.80              |
| 1:1A:985:C:N3      | 1:1A:1068:G:N1     | 2.25                     | 0.80              |
| 12:2D:76:MET:CE    | 12:2D:148:VAL:HG12 | 2.11                     | 0.80              |
| 47:2m:928:G:H2'    | 47:2m:929:G:C8     | 2.16                     | 0.80              |
| 55:2u:15:LEU:HD13  | 55:2u:49:MET:HE1   | 1.63                     | 0.80              |
| 1:1A:417:G:H1'     | 1:1A:418:A:OP2     | 1.81                     | 0.80              |
| 1:1A:1438:U:H3'    | 1:1A:1439:C:C5'    | 2.11                     | 0.80              |
| 47:2m:338:G:O2'    | 47:2m:339:A:H5'    | 1.81                     | 0.80              |
| 9:2A:221:LYS:O     | 9:2A:221:LYS:HG3   | 1.80                     | 0.80              |
| 47:2m:944:A:H5'    | 74:3L:134:PRO:HB3  | 1.64                     | 0.80              |
| 60:2z:42:HIS:O     | 60:2z:46:ARG:HG2   | 1.81                     | 0.80              |
| 68:3F:286:CYS:HA   | 68:3F:302:TYR:HA   | 1.64                     | 0.80              |
| 21:2M:96:GLU:HG3   | 21:2M:139:ARG:HG2  | 1.63                     | 0.80              |
| 47:2m:525:A:H2'    | 47:2m:526:A:H8     | 1.44                     | 0.80              |
| 47:2m:875:A:H5'    | 53:2s:111:LYS:CE   | 2.11                     | 0.80              |
| 47:2m:957:A:H2'    | 47:2m:958:G:N2     | 1.97                     | 0.80              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 47:2m:1598:G:O2'     | 77:3O:80:ARG:O     | 1.98                     | 0.80              |
| 47:2m:1677:U:OP1     | 52:2r:148:ASN:ND2  | 2.14                     | 0.80              |
| 48:2n:159:ILE:HD11   | 63:3A:34:MET:CE    | 2.10                     | 0.80              |
| 1:1A:74:G:H5'        | 14:2F:59:VAL:HG13  | 1.62                     | 0.80              |
| 1:1A:136:C:H4'       | 1:1A:137:G:N7      | 1.96                     | 0.80              |
| 1:1A:1933:G:H2'      | 1:1A:1934:A:C8     | 2.16                     | 0.80              |
| 1:1A:2768:C:H3'      | 1:1A:2769:U:H5'    | 1.63                     | 0.80              |
| 47:2m:688:U:H4'      | 47:2m:689:U:O5'    | 1.82                     | 0.80              |
| 48:2n:198:MET:HG2    | 48:2n:199:PRO:HD2  | 1.61                     | 0.80              |
| 49:2o:69:VAL:HG13    | 49:2o:74:LEU:HD11  | 1.61                     | 0.80              |
| 72:3J:22:LEU:HD21    | 72:3J:89:VAL:HA    | 1.63                     | 0.80              |
| 78:3P:81:ARG:HD3     | 78:3P:84:HIS:HA    | 1.63                     | 0.80              |
| 6:1F:8:ILE:HD11      | 6:1F:153:VAL:HG23  | 1.63                     | 0.80              |
| 25:2Q:91:MET:HA      | 25:2Q:91:MET:HE3   | 1.63                     | 0.80              |
| 26:2R:87:MET:O       | 26:2R:91:GLU:HG3   | 1.80                     | 0.80              |
| 47:2m:292:A:OP2      | 56:2v:42:LEU:HD21  | 1.82                     | 0.80              |
| 47:2m:496:C:H5'      | 51:2q:29:PRO:HA    | 1.63                     | 0.80              |
| 49:2o:89:GLU:OE2     | 49:2o:220:LYS:NZ   | 2.14                     | 0.80              |
| 68:3F:68:ASP:OD2     | 68:3F:111:VAL:N    | 2.15                     | 0.80              |
| 78:3P:42:LYS:HD2     | 78:3P:57:VAL:HB    | 1.64                     | 0.80              |
| 1:1A:1218:G:H3'      | 1:1A:1219:G:H5''   | 1.61                     | 0.80              |
| 1:1A:3596:A:H2'      | 1:1A:3597:G:H5'    | 1.64                     | 0.80              |
| 4:1D:28:ARG:HB2      | 4:1D:123:ARG:HB2   | 1.62                     | 0.80              |
| 9:2A:95:ILE:O        | 9:2A:223:LYS:HD2   | 1.81                     | 0.80              |
| 1:1A:280:G:H5''      | 16:2H:14:LYS:HE2   | 1.63                     | 0.80              |
| 1:1A:1437:C:O2'      | 1:1A:1438:U:H5'    | 1.82                     | 0.80              |
| 1:1A:4587:G:OP1      | 17:2I:61:ARG:HD2   | 1.81                     | 0.80              |
| 1:1A:4591:U:H2'      | 1:1A:4592:C:C6     | 2.17                     | 0.80              |
| 1:1A:4678:G:N2       | 1:1A:4713:G:H1'    | 1.96                     | 0.80              |
| 9:2A:116:GLN:O       | 9:2A:119:ASN:HB2   | 1.82                     | 0.80              |
| 10:2B:137[B]:ARG:HD3 | 10:2B:146:LEU:HD11 | 1.63                     | 0.80              |
| 26:2R:80:PRO:HG2     | 26:2R:155:ILE:HG21 | 1.64                     | 0.80              |
| 47:2m:744:G:O2'      | 47:2m:746:C:O4'    | 2.00                     | 0.80              |
| 47:2m:1016:U:OP1     | 78:3P:30:SER:OG    | 1.99                     | 0.80              |
| 47:2m:1236:G:O6      | 60:2z:137:LYS:NZ   | 2.14                     | 0.80              |
| 52:2r:127:ARG:HG2    | 52:2r:137:GLN:HB2  | 1.62                     | 0.80              |
| 52:2r:167:LYS:NZ     | 52:2r:175:ASP:OD2  | 2.13                     | 0.80              |
| 60:2z:5:ILE:HD12     | 60:2z:6:PRO:CD     | 2.11                     | 0.80              |
| 72:3J:44:LYS:NZ      | 80:3R:127:GLY:O    | 2.15                     | 0.80              |
| 1:1A:705:G:OP2       | 33:2Y:5:ARG:NH2    | 2.14                     | 0.80              |
| 10:2B:58:PRO:HG2     | 10:2B:61:ILE:HD12  | 1.64                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:2W:28:VAL:CG1   | 31:2W:33:GLN:HB3   | 2.12                     | 0.80              |
| 46:2l:198:TRP:CZ2  | 46:2l:202:ARG:HB2  | 2.16                     | 0.80              |
| 47:2m:1291:A:N6    | 47:2m:1308:U:O4    | 2.15                     | 0.80              |
| 5:1E:160:ILE:HD11  | 5:1E:194:LEU:HD12  | 1.62                     | 0.79              |
| 52:2r:121:PRO:HB3  | 52:2r:193:LYS:HG2  | 1.64                     | 0.79              |
| 68:3F:110:SER:HB2  | 68:3F:155:ARG:HH22 | 1.47                     | 0.79              |
| 68:3F:120:ILE:HG22 | 68:3F:132:TRP:HB2  | 1.62                     | 0.79              |
| 69:3G:102:LEU:HB3  | 69:3G:130:ILE:HD11 | 1.64                     | 0.79              |
| 1:1A:406:C:O2'     | 1:1A:407:A:OP1     | 1.98                     | 0.79              |
| 1:1A:922:C:H2'     | 1:1A:923:C:O4'     | 1.81                     | 0.79              |
| 47:2m:1568:C:OP1   | 61:20:96:SER:OG    | 1.98                     | 0.79              |
| 53:2s:7:LYS:NZ     | 53:2s:20:GLU:O     | 2.14                     | 0.79              |
| 71:3I:107:GLU:O    | 71:3I:112:THR:OG1  | 2.00                     | 0.79              |
| 1:1A:1366:G:H2'    | 1:1A:1367:C:H5''   | 1.65                     | 0.79              |
| 8:1H:128:HIS:ND1   | 8:1H:128:HIS:O     | 2.16                     | 0.79              |
| 48:2n:163:CYS:SG   | 48:2n:174:MET:HG2  | 2.22                     | 0.79              |
| 47:2m:907:G:H2'    | 47:2m:908:A:C8     | 2.17                     | 0.79              |
| 47:2m:1271:C:H2'   | 67:3E:2:GLY:HA2    | 1.62                     | 0.79              |
| 47:2m:1280:G:O6    | 47:2m:1317:C:N4    | 2.15                     | 0.79              |
| 48:2n:77:ILE:HD12  | 48:2n:99:ILE:HB    | 1.63                     | 0.79              |
| 57:2w:115:TYR:N    | 57:2w:118:GLU:OE2  | 2.15                     | 0.79              |
| 76:3N:106:GLN:HA   | 76:3N:109:GLU:CD   | 2.08                     | 0.79              |
| 1:1A:216:C:H3'     | 1:1A:217:C:H5''    | 1.64                     | 0.79              |
| 1:1A:308:G:OP2     | 1:1A:308:G:N2      | 2.13                     | 0.79              |
| 1:1A:2858:A:O2'    | 1:1A:2859:G:H5'    | 1.82                     | 0.79              |
| 47:2m:1420:G:N2    | 47:2m:1427:C:O2'   | 2.14                     | 0.79              |
| 53:2s:20:GLU:OE1   | 53:2s:23:ILE:HD12  | 1.82                     | 0.79              |
| 54:2t:172:LEU:HD13 | 54:2t:190:LEU:HD12 | 1.65                     | 0.79              |
| 59:2y:30:THR:O     | 59:2y:34:VAL:HG23  | 1.82                     | 0.79              |
| 5:1E:224:LYS:HG2   | 5:1E:340:THR:HG22  | 1.65                     | 0.79              |
| 39:2e:12:LEU:O     | 39:2e:16:ARG:HG2   | 1.83                     | 0.79              |
| 47:2m:799:U:O4     | 47:2m:867:G:N2     | 2.16                     | 0.79              |
| 47:2m:958:G:H2'    | 47:2m:959:G:C8     | 2.17                     | 0.79              |
| 47:2m:1403:C:N4    | 47:2m:1437:C:OP2   | 2.16                     | 0.79              |
| 50:2p:68:GLU:HB2   | 55:2u:20:VAL:CG1   | 2.12                     | 0.79              |
| 72:3J:24:THR:O     | 72:3J:27:ILE:HG22  | 1.81                     | 0.79              |
| 47:2m:65:C:N4      | 70:3H:134:GLY:O    | 2.16                     | 0.79              |
| 47:2m:1301:A:H2'   | 47:2m:1303:C:C6    | 2.18                     | 0.79              |
| 53:2s:8:ILE:HD12   | 53:2s:9:VAL:H      | 1.48                     | 0.79              |
| 60:2z:39:ARG:O     | 60:2z:43:VAL:HG12  | 1.82                     | 0.79              |
| 71:3I:137:VAL:HG12 | 71:3I:138[A]:ARG:H | 1.47                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:3I:137:VAL:HG12 | 71:3I:138[B]:ARG:H | 1.47                     | 0.79              |
| 77:3O:47:LEU:HG    | 77:3O:83:LEU:HD12  | 1.63                     | 0.79              |
| 1:1A:989:U:O2'     | 1:1A:990:C:O4'     | 1.99                     | 0.79              |
| 1:1A:1439:C:OP2    | 9:2A:31:LYS:NZ     | 2.15                     | 0.79              |
| 3:1C:55:U:H3       | 3:1C:62:A:H2       | 1.28                     | 0.79              |
| 51:2q:107:GLY:HA2  | 51:2q:189:LEU:HG   | 1.64                     | 0.79              |
| 55:2u:13:GLU:HG3   | 55:2u:14:LEU:HD22  | 1.62                     | 0.79              |
| 1:1A:911:U:H2'     | 1:1A:912:G:O4'     | 1.83                     | 0.79              |
| 11:2C:51:LYS:H     | 11:2C:51:LYS:HD3   | 1.48                     | 0.79              |
| 47:2m:224:A:H2'    | 47:2m:225:G:O4'    | 1.81                     | 0.79              |
| 1:1A:4901:G:H3'    | 1:1A:4901:G:OP1    | 1.83                     | 0.79              |
| 46:2l:91:LYS:HA    | 46:2l:124:LEU:HD23 | 1.65                     | 0.79              |
| 47:2m:291:G:H5''   | 51:2q:203:GLY:H    | 1.48                     | 0.79              |
| 47:2m:1235:G:H21   | 57:2w:135:ALA:HB2  | 1.47                     | 0.79              |
| 47:2m:1480:A:O2'   | 67:3E:56:ASP:OXT   | 1.98                     | 0.79              |
| 54:2t:129:LEU:HB3  | 54:2t:133:GLU:HB2  | 1.63                     | 0.79              |
| 70:3H:50:VAL:CG2   | 70:3H:111:LEU:HB3  | 2.13                     | 0.79              |
| 7:1G:86:TYR:CE1    | 7:1G:247:ILE:HG13  | 2.18                     | 0.78              |
| 35:2a:99:GLU:O     | 35:2a:103:VAL:HG13 | 1.83                     | 0.78              |
| 47:2m:145:G:H2'    | 47:2m:146:G:C8     | 2.18                     | 0.78              |
| 69:3G:74:LYS:HE3   | 69:3G:269:PHE:CB   | 2.12                     | 0.78              |
| 77:3O:87:ALA:O     | 77:3O:90:GLU:HG3   | 1.83                     | 0.78              |
| 77:3O:98:LYS:HG2   | 77:3O:110:THR:HG23 | 1.64                     | 0.78              |
| 23:2O:48:LYS:HG2   | 23:2O:53:ALA:HB2   | 1.62                     | 0.78              |
| 31:2W:77:ASN:OD1   | 31:2W:80:GLU:HG3   | 1.82                     | 0.78              |
| 50:2p:127:MET:CE   | 50:2p:134:CYS:HB3  | 2.12                     | 0.78              |
| 60:2z:44:VAL:HB    | 60:2z:70:ILE:CD1   | 2.13                     | 0.78              |
| 61:20:23:LYS:HA    | 61:20:54:TYR:HE2   | 1.48                     | 0.78              |
| 70:3H:18:VAL:HG11  | 70:3H:24:LEU:HD21  | 1.63                     | 0.78              |
| 1:1A:455:C:O2'     | 1:1A:456:C:H5'     | 1.83                     | 0.78              |
| 1:1A:2448:G:H2'    | 1:1A:2449:A:C8     | 2.19                     | 0.78              |
| 1:1A:4061:G:O2'    | 1:1A:4062:A:O4'    | 2.02                     | 0.78              |
| 23:2O:67:LYS:HD2   | 23:2O:67:LYS:O     | 1.82                     | 0.78              |
| 36:2b:4:ILE:HD13   | 36:2b:9:LEU:HD11   | 1.65                     | 0.78              |
| 47:2m:870:A:OP1    | 47:2m:870:A:H2'    | 1.83                     | 0.78              |
| 47:2m:1269:G:N2    | 47:2m:1298:G:O6    | 2.16                     | 0.78              |
| 47:2m:1620:A:OP1   | 57:2w:115:TYR:OH   | 2.01                     | 0.78              |
| 51:2q:55:ALA:HB3   | 51:2q:61:VAL:HG22  | 1.66                     | 0.78              |
| 52:2r:87:LEU:HG    | 58:2x:46:THR:HB    | 1.65                     | 0.78              |
| 68:3F:79:LEU:HD13  | 68:3F:120:ILE:HG12 | 1.64                     | 0.78              |
| 69:3G:152:ARG:O    | 69:3G:156:ILE:HG23 | 1.84                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:253:G:H2'     | 1:1A:254:G:O4'     | 1.84                     | 0.78              |
| 1:1A:1272:C:H5''   | 9:2A:34:ARG:HG2    | 1.64                     | 0.78              |
| 1:1A:4773:C:H2'    | 1:1A:4774:C:C6     | 2.18                     | 0.78              |
| 11:2C:24:THR:OG1   | 11:2C:37:ASP:OD1   | 2.00                     | 0.78              |
| 47:2m:149:A:H3'    | 47:2m:150:A:H8     | 1.48                     | 0.78              |
| 47:2m:611:G:H2'    | 47:2m:612:U:H6     | 1.49                     | 0.78              |
| 47:2m:693:A:C2'    | 47:2m:694:G:H5''   | 2.14                     | 0.78              |
| 47:2m:1217:A:H2'   | 47:2m:1218:C:C6    | 2.19                     | 0.78              |
| 58:2x:32:ILE:HD12  | 58:2x:68:ILE:CB    | 2.12                     | 0.78              |
| 60:2z:38:ARG:O     | 60:2z:42:HIS:ND1   | 2.16                     | 0.78              |
| 60:2z:70:ILE:HG22  | 60:2z:77:TYR:CD2   | 2.19                     | 0.78              |
| 77:3O:99:LEU:CD2   | 77:3O:102:LYS:HB3  | 2.08                     | 0.78              |
| 1:1A:2111:G:N1     | 1:1A:2252:G:O4'    | 2.15                     | 0.78              |
| 1:1A:4880:C:O2'    | 1:1A:4881:U:H5'    | 1.83                     | 0.78              |
| 17:2I:54:TYR:CD1   | 17:2I:145:VAL:HG21 | 2.18                     | 0.78              |
| 50:2p:76:ARG:CG    | 55:2u:22:VAL:HG11  | 2.13                     | 0.78              |
| 72:3J:67:ALA:HB2   | 80:3R:108:VAL:HG23 | 1.65                     | 0.78              |
| 72:3J:126:GLU:O    | 72:3J:129:LYS:HG3  | 1.82                     | 0.78              |
| 1:1A:2254:G:H4'    | 1:1A:2255:C:C5     | 2.19                     | 0.78              |
| 21:2M:95:ARG:NH2   | 21:2M:112:ASP:OD2  | 2.15                     | 0.78              |
| 47:2m:549:C:HO2'   | 47:2m:550:C:P      | 2.06                     | 0.78              |
| 47:2m:1215:C:H42   | 47:2m:1220:A:N6    | 1.79                     | 0.78              |
| 54:2t:139:LYS:HB2  | 54:2t:141:ARG:HD3  | 1.63                     | 0.78              |
| 67:3E:22:ARG:NH1   | 67:3E:36:LEU:O     | 2.15                     | 0.78              |
| 1:1A:1375:C:O2'    | 1:1A:1376:C:H5'    | 1.84                     | 0.78              |
| 1:1A:4459:U:H2'    | 1:1A:4460:U:C6     | 2.19                     | 0.78              |
| 9:2A:114:LEU:HD21  | 9:2A:121:THR:HG22  | 1.66                     | 0.78              |
| 11:2C:165:THR:HG21 | 11:2C:179:ILE:HD12 | 1.66                     | 0.78              |
| 47:2m:191:A:N6     | 47:2m:208:G:O2'    | 2.17                     | 0.78              |
| 49:2o:36:PRO:HB2   | 49:2o:38:MET:SD    | 2.24                     | 0.78              |
| 57:2w:98:ASN:HD21  | 57:2w:100:LYS:HE2  | 1.47                     | 0.78              |
| 62:21:41:ARG:HA    | 62:21:44:LYS:HE2   | 1.65                     | 0.78              |
| 1:1A:397:G:H2'     | 1:1A:398:A:H5'     | 1.64                     | 0.78              |
| 1:1A:3596:A:H1'    | 56:2v:2:ALA:HA     | 1.64                     | 0.78              |
| 47:2m:138:C:H5''   | 47:2m:139:C:H5     | 1.49                     | 0.78              |
| 48:2n:111:GLN:HA   | 48:2n:116:PHE:CE2  | 2.19                     | 0.78              |
| 1:1A:499:G:O2'     | 1:1A:500:G:OP1     | 2.02                     | 0.78              |
| 1:1A:2744:A:H2'    | 1:1A:2745:A:C8     | 2.18                     | 0.78              |
| 3:1C:21:C:O2'      | 3:1C:22:U:H5'      | 1.83                     | 0.78              |
| 16:2H:60:VAL:HG22  | 16:2H:134:LEU:HB2  | 1.66                     | 0.78              |
| 46:2l:86:ASP:HB3   | 46:2l:88:GLU:OE2   | 1.82                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1139:C:H2'   | 47:2m:1140:G:O4'   | 1.84                     | 0.78              |
| 48:2n:5:LEU:HD13   | 63:3A:41:LYS:HA    | 1.66                     | 0.78              |
| 58:2x:40:GLU:HG3   | 58:2x:41:MET:SD    | 2.24                     | 0.78              |
| 71:3I:124:HIS:CE1  | 79:3Q:35:ARG:HG3   | 2.18                     | 0.78              |
| 1:1A:1669:A:H4'    | 1:1A:1685:G:N2     | 1.99                     | 0.78              |
| 1:1A:4104:G:H2'    | 1:1A:4106:G:H21    | 1.48                     | 0.78              |
| 10:2B:99:ALA:HB1   | 10:2B:136:LEU:HD11 | 1.66                     | 0.78              |
| 51:2q:73:ASP:HA    | 51:2q:164:LEU:HD13 | 1.65                     | 0.78              |
| 57:2w:93:MET:HE1   | 57:2w:104:GLN:HB3  | 1.65                     | 0.78              |
| 70:3H:63:MET:HA    | 70:3H:63:MET:CE    | 2.14                     | 0.78              |
| 72:3J:36:ARG:NH1   | 72:3J:36:ARG:O     | 2.17                     | 0.78              |
| 23:2O:42:PHE:CE2   | 23:2O:90:TYR:HB2   | 2.19                     | 0.77              |
| 47:2m:3:C:O2       | 71:3I:18:ARG:NH2   | 2.12                     | 0.77              |
| 47:2m:629:A:O2'    | 47:2m:631:U:OP1    | 2.02                     | 0.77              |
| 47:2m:1408:U:O2    | 58:2x:71:ARG:NH2   | 2.17                     | 0.77              |
| 53:2s:31:GLU:HB2   | 53:2s:32:MET:CE    | 2.13                     | 0.77              |
| 1:1A:1332:C:H2'    | 1:1A:1333:A:H8     | 1.49                     | 0.77              |
| 1:1A:1817:U:O2'    | 1:1A:1818:G:H5'    | 1.83                     | 0.77              |
| 1:1A:3726:A:O2'    | 1:1A:3727:A:O5'    | 2.02                     | 0.77              |
| 47:2m:54:A:OP1     | 76:3N:111:LYS:NZ   | 2.14                     | 0.77              |
| 47:2m:611:G:H2'    | 47:2m:612:U:C6     | 2.18                     | 0.77              |
| 47:2m:1415:C:H2'   | 47:2m:1417:C:H4'   | 1.64                     | 0.77              |
| 50:2p:69:LEU:HD22  | 50:2p:86:LEU:CD1   | 2.14                     | 0.77              |
| 65:3C:45:VAL:HG21  | 65:3C:64:LEU:HD12  | 1.65                     | 0.77              |
| 68:3F:118:ARG:HD3  | 68:3F:119:GLN:OE1  | 1.84                     | 0.77              |
| 68:3F:154:VAL:HG13 | 68:3F:167:SER:HB3  | 1.65                     | 0.77              |
| 1:1A:483:G:H3'     | 1:1A:484:U:H5'     | 1.66                     | 0.77              |
| 1:1A:2669:C:O2'    | 1:1A:2670:C:H6     | 1.67                     | 0.77              |
| 1:1A:2764:A:H2'    | 1:1A:2765:A:H8     | 1.50                     | 0.77              |
| 47:2m:534:G:H2'    | 47:2m:535:G:C8     | 2.20                     | 0.77              |
| 47:2m:550:C:O2'    | 47:2m:551:U:O5'    | 2.01                     | 0.77              |
| 47:2m:1112:U:C2'   | 47:2m:1113:A:H4'   | 2.11                     | 0.77              |
| 53:2s:31:GLU:HB3   | 53:2s:37:LYS:NZ    | 1.99                     | 0.77              |
| 69:3G:132:ASP:OD1  | 69:3G:134:ASN:N    | 2.17                     | 0.77              |
| 76:3N:36:PRO:O     | 76:3N:40:ILE:HG13  | 1.83                     | 0.77              |
| 1:1A:216:C:H3'     | 1:1A:217:C:C5'     | 2.15                     | 0.77              |
| 1:1A:2092:G:O2'    | 1:1A:2262:G:N2     | 2.17                     | 0.77              |
| 1:1A:4061:G:H2'    | 1:1A:4062:A:C8     | 2.19                     | 0.77              |
| 13:2E:31:ASP:HA    | 13:2E:34:THR:HG22  | 1.64                     | 0.77              |
| 47:2m:71:G:H3'     | 47:2m:72:C:H5''    | 1.66                     | 0.77              |
| 47:2m:1276:A:H62   | 47:2m:1321:G:H8    | 1.30                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:2n:23:THR:HG23  | 48:2n:163:CYS:HB2  | 1.65                     | 0.77              |
| 53:2s:8:ILE:HD12   | 53:2s:9:VAL:N      | 1.99                     | 0.77              |
| 54:2t:119:LEU:HD21 | 54:2t:153:LYS:HD3  | 1.65                     | 0.77              |
| 62:21:80:PHE:HB3   | 67:3E:52:PHE:HB3   | 1.67                     | 0.77              |
| 47:2m:1554:C:H5'   | 47:2m:1555:U:C1'   | 2.15                     | 0.77              |
| 71:3I:78:LEU:HD21  | 71:3I:97:ILE:HD11  | 1.64                     | 0.77              |
| 77:3O:47:LEU:HD22  | 77:3O:79:ILE:HG23  | 1.65                     | 0.77              |
| 1:1A:661:C:H2'     | 1:1A:662:C:C6      | 2.20                     | 0.77              |
| 1:1A:4730:C:H5'    | 1:1A:4965:U:O2     | 1.84                     | 0.77              |
| 47:2m:980:A:H2'    | 47:2m:981:A:C8     | 2.20                     | 0.77              |
| 47:2m:1617:G:N1    | 47:2m:1620:A:OP2   | 2.18                     | 0.77              |
| 31:2W:21:VAL:HG11  | 31:2W:96:ILE:HD12  | 1.67                     | 0.77              |
| 47:2m:907:G:O2'    | 47:2m:908:A:O5'    | 2.01                     | 0.77              |
| 47:2m:1413:G:N1    | 47:2m:1433:C:O2    | 2.16                     | 0.77              |
| 1:1A:2079:G:OP2    | 33:2Y:64:LYS:NZ    | 2.17                     | 0.77              |
| 46:2l:29:LEU:HD21  | 46:2l:173:LYS:HB3  | 1.67                     | 0.77              |
| 60:2z:31:THR:HA    | 60:2z:36:VAL:HG12  | 1.66                     | 0.77              |
| 1:1A:1893:C:H1'    | 1:1A:1937:C:O2     | 1.85                     | 0.77              |
| 1:1A:4694:G:H4'    | 11:2C:71:ARG:HH12  | 1.48                     | 0.77              |
| 47:2m:165:G:N2     | 47:2m:165:G:OP2    | 2.18                     | 0.77              |
| 47:2m:984:C:O2'    | 74:3L:138:ASP:O    | 2.01                     | 0.77              |
| 47:2m:1215:C:O2'   | 47:2m:1645:C:OP2   | 2.01                     | 0.77              |
| 58:2x:32:ILE:HD12  | 58:2x:68:ILE:HB    | 1.66                     | 0.77              |
| 1:1A:3873:G:H2'    | 1:1A:3874:G:C8     | 2.20                     | 0.77              |
| 7:1G:103:LEU:HG    | 7:1G:247:ILE:HG21  | 1.66                     | 0.77              |
| 8:1H:161:ARG:NH1   | 8:1H:273:SER:OG    | 2.18                     | 0.77              |
| 47:2m:1507:G:O2'   | 47:2m:1508:A:H5'   | 1.85                     | 0.77              |
| 77:3O:73:VAL:HG11  | 77:3O:88:LEU:HD11  | 1.65                     | 0.77              |
| 1:1A:496:G:N1      | 1:1A:658:C:O2      | 2.17                     | 0.76              |
| 1:1A:3773:U:O2'    | 1:1A:3774:A:OP2    | 2.03                     | 0.76              |
| 47:2m:1217:A:H2'   | 47:2m:1218:C:H6    | 1.50                     | 0.76              |
| 50:2p:66:ILE:O     | 50:2p:70:THR:HG23  | 1.86                     | 0.76              |
| 51:2q:122:LYS:HG2  | 51:2q:162:ILE:HD11 | 1.67                     | 0.76              |
| 1:1A:4076:G:OP1    | 10:2B:73:ARG:NE    | 2.11                     | 0.76              |
| 4:1D:14:SER:HA     | 4:1D:17:ARG:HE     | 1.49                     | 0.76              |
| 5:1E:56:ILE:HD13   | 5:1E:365:LEU:HD22  | 1.67                     | 0.76              |
| 11:2C:106:GLN:NE2  | 11:2C:113:GLU:OE1  | 2.16                     | 0.76              |
| 22:2N:157:GLU:HG2  | 22:2N:159:MET:HE2  | 1.66                     | 0.76              |
| 25:2Q:80:ARG:NH2   | 70:3H:129:VAL:O    | 2.18                     | 0.76              |
| 47:2m:443:U:H2'    | 47:2m:444:G:O4'    | 1.86                     | 0.76              |
| 47:2m:465:A:H4'    | 47:2m:466:G:O5'    | 1.84                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1221:G:O2'   | 47:2m:1676:U:O2    | 2.03                     | 0.76              |
| 60:2z:10:GLN:HE21  | 60:2z:57:GLY:HA2   | 1.51                     | 0.76              |
| 61:20:130:ASP:O    | 61:20:134:ILE:HG23 | 1.85                     | 0.76              |
| 71:3l:42:GLU:O     | 71:3l:46:VAL:HG23  | 1.84                     | 0.76              |
| 1:1A:93:G:H2'      | 1:1A:94:A:C8       | 2.20                     | 0.76              |
| 50:2p:217:ILE:HG23 | 50:2p:218:LEU:HD23 | 1.66                     | 0.76              |
| 51:2q:159:THR:HB   | 51:2q:173:ILE:CG1  | 2.15                     | 0.76              |
| 54:2t:56:ARG:HB2   | 54:2t:180:GLY:HA2  | 1.67                     | 0.76              |
| 75:3M:49:GLU:O     | 75:3M:64:ASN:ND2   | 2.17                     | 0.76              |
| 1:1A:513:U:H3'     | 1:1A:514:U:H4'     | 1.68                     | 0.76              |
| 1:1A:985:C:O2      | 1:1A:1068:G:N2     | 2.15                     | 0.76              |
| 1:1A:1973:G:H3'    | 1:1A:1974:U:H5'    | 1.67                     | 0.76              |
| 1:1A:4635:A:H2     | 1:1A:4663:G:H21    | 1.30                     | 0.76              |
| 14:2F:81:LEU:HD11  | 14:2F:98:VAL:HG22  | 1.66                     | 0.76              |
| 46:2l:159:MET:HA   | 46:2l:165:LEU:HD21 | 1.68                     | 0.76              |
| 47:2m:656:G:N2     | 47:2m:663:C:H5''   | 1.99                     | 0.76              |
| 47:2m:1119:A:O3'   | 78:3P:72:ARG:NH2   | 2.18                     | 0.76              |
| 47:2m:1308:U:O2'   | 80:3R:134:SER:N    | 2.19                     | 0.76              |
| 49:2o:144:LYS:HD3  | 49:2o:208:HIS:HB3  | 1.67                     | 0.76              |
| 1:1A:1081:C:O2'    | 1:1A:1219:G:N2     | 2.18                     | 0.76              |
| 1:1A:1363:C:H3'    | 14:2F:36:ARG:HH22  | 1.49                     | 0.76              |
| 1:1A:2840:A:O2'    | 1:1A:2841:G:H5'    | 1.85                     | 0.76              |
| 17:2l:27:VAL:HG13  | 17:2l:98:ALA:HB1   | 1.66                     | 0.76              |
| 31:2W:23:LYS:O     | 31:2W:23:LYS:HD2   | 1.86                     | 0.76              |
| 47:2m:1159:G:OP2   | 64:3B:5:ARG:NH1    | 2.18                     | 0.76              |
| 80:3R:119:ARG:O    | 80:3R:132:MET:N    | 2.19                     | 0.76              |
| 1:1A:106:A:H1'     | 1:1A:336:A:H8      | 1.50                     | 0.76              |
| 1:1A:2261:G:H5''   | 8:1H:112:MET:HE2   | 1.67                     | 0.76              |
| 12:2D:180:GLU:HG3  | 12:2D:184:MET:CE   | 2.16                     | 0.76              |
| 47:2m:1475:G:O2'   | 47:2m:1476:A:OP2   | 2.02                     | 0.76              |
| 50:2p:33:GLY:HA3   | 50:2p:53:THR:HG23  | 1.68                     | 0.76              |
| 51:2q:88:ASP:OD1   | 51:2q:122:LYS:NZ   | 2.13                     | 0.76              |
| 54:2t:190:LEU:HD22 | 54:2t:194:GLU:HG3  | 1.67                     | 0.76              |
| 57:2w:23:ASP:OD1   | 57:2w:24:GLN:N     | 2.19                     | 0.76              |
| 61:20:38:LYS:HD3   | 61:20:41:LYS:HB3   | 1.68                     | 0.76              |
| 70:3H:199:THR:HG22 | 70:3H:203:LYS:HE3  | 1.66                     | 0.76              |
| 70:3H:221:LYS:O    | 70:3H:224:ARG:HG2  | 1.84                     | 0.76              |
| 76:3N:121:ALA:O    | 76:3N:125:VAL:HG23 | 1.85                     | 0.76              |
| 1:1A:1345:A:H2'    | 1:1A:1346:C:C6     | 2.20                     | 0.76              |
| 1:1A:1720:C:H2'    | 1:1A:1721:G:O4'    | 1.85                     | 0.76              |
| 1:1A:3971:G:O6     | 1:1A:4049:U:H5'    | 1.85                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1778:C:H2'   | 47:2m:1779:G:C8    | 2.20                     | 0.76              |
| 48:2n:155:ARG:HG2  | 48:2n:156:TYR:CD2  | 2.21                     | 0.76              |
| 49:2o:133:TYR:O    | 49:2o:135:LEU:HG   | 1.86                     | 0.76              |
| 69:3G:174:ILE:HD12 | 69:3G:174:ILE:O    | 1.85                     | 0.76              |
| 73:3K:29:THR:O     | 73:3K:33:VAL:HG23  | 1.86                     | 0.76              |
| 1:1A:711:A:H2'     | 1:1A:712:C:C6      | 2.19                     | 0.76              |
| 49:2o:57:ILE:HB    | 49:2o:60:ASP:OD1   | 1.86                     | 0.76              |
| 55:2u:24:LYS:HG3   | 55:2u:26:ASP:OD1   | 1.86                     | 0.76              |
| 1:1A:655:C:OP2     | 6:1F:268:ARG:NH2   | 2.19                     | 0.76              |
| 1:1A:737:C:H3'     | 1:1A:738:C:H5'     | 1.66                     | 0.76              |
| 11:2C:31:ARG:NH1   | 11:2C:149:ASN:OD1  | 2.19                     | 0.76              |
| 47:2m:160:U:O2'    | 47:2m:161:U:H5'    | 1.86                     | 0.76              |
| 47:2m:419:G:H4'    | 75:3M:88:LYS:HD2   | 1.67                     | 0.76              |
| 47:2m:561:A:OP2    | 71:3I:174:LYS:HB2  | 1.86                     | 0.76              |
| 47:2m:1208:A:OP2   | 47:2m:1835:A:O2'   | 2.04                     | 0.76              |
| 52:2r:96:ALA:O     | 52:2r:100:ILE:HG12 | 1.85                     | 0.76              |
| 73:3K:63:VAL:HA    | 73:3K:66:VAL:CG1   | 2.16                     | 0.76              |
| 76:3N:16:ARG:H     | 76:3N:16:ARG:HD2   | 1.51                     | 0.76              |
| 47:2m:1101:U:H2'   | 47:2m:1102:G:C8    | 2.21                     | 0.76              |
| 47:2m:1257:G:H4'   | 47:2m:1258:A:H5'   | 1.67                     | 0.76              |
| 47:2m:1595:U:H2'   | 47:2m:1596:U:C6    | 2.20                     | 0.76              |
| 47:2m:1751:C:O2    | 47:2m:1782:G:N1    | 2.19                     | 0.76              |
| 72:3J:42:LEU:HD13  | 72:3J:69:LEU:HD21  | 1.68                     | 0.76              |
| 1:1A:2055:G:H4'    | 1:1A:2056:G:OP2    | 1.84                     | 0.75              |
| 1:1A:4708:A:N3     | 1:1A:4709:U:H5'    | 2.02                     | 0.75              |
| 11:2C:137:SER:HB3  | 11:2C:143:GLU:HG3  | 1.69                     | 0.75              |
| 80:3R:120:GLU:HA   | 80:3R:131:PHE:HA   | 1.69                     | 0.75              |
| 1:1A:5053:U:H3'    | 1:1A:5054:C:C6     | 2.21                     | 0.75              |
| 5:1E:117:ARG:HA    | 5:1E:177:LYS:HD2   | 1.66                     | 0.75              |
| 51:2q:98:ASN:O     | 51:2q:114:ILE:HG12 | 1.85                     | 0.75              |
| 51:2q:181:CYS:HB3  | 51:2q:195:ILE:HD11 | 1.66                     | 0.75              |
| 51:2q:208:VAL:CG1  | 51:2q:225:ILE:HG13 | 2.16                     | 0.75              |
| 52:2r:92:ILE:HD12  | 52:2r:169:ILE:HG23 | 1.68                     | 0.75              |
| 69:3G:92:GLU:HA    | 69:3G:95:ASP:OD1   | 1.86                     | 0.75              |
| 1:1A:4094:G:H2'    | 1:1A:4095:G:C8     | 2.22                     | 0.75              |
| 12:2D:87:MET:HG2   | 12:2D:138:ILE:HG12 | 1.69                     | 0.75              |
| 14:2F:139:SER:OG   | 14:2F:142:GLU:OE1  | 2.02                     | 0.75              |
| 47:2m:67:C:H1'     | 47:2m:69:C:OP2     | 1.86                     | 0.75              |
| 47:2m:942:G:H2'    | 47:2m:943:U:C6     | 2.22                     | 0.75              |
| 47:2m:1278:A:H2'   | 47:2m:1279:C:C6    | 2.21                     | 0.75              |
| 55:2u:24:LYS:O     | 55:2u:42:ASN:ND2   | 2.19                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:3L:100:THR:HG21 | 74:3L:104:ARG:HD3  | 1.68                     | 0.75              |
| 1:1A:1199:G:H2'    | 1:1A:1200:G:C8     | 2.21                     | 0.75              |
| 1:1A:4046:A:OP1    | 1:1A:4046:A:H3'    | 1.86                     | 0.75              |
| 2:1B:109:U:H4'     | 2:1B:110:G:OP2     | 1.87                     | 0.75              |
| 31:2W:22:MET:O     | 31:2W:23:LYS:HG3   | 1.87                     | 0.75              |
| 37:2c:43:MET:HA    | 37:2c:43:MET:HE3   | 1.69                     | 0.75              |
| 47:2m:1849:G:HO2'  | 47:2m:1850:A:H8    | 1.35                     | 0.75              |
| 58:2x:48:GLN:O     | 58:2x:52:LEU:HG    | 1.86                     | 0.75              |
| 59:2y:13:ALA:O     | 59:2y:17:ILE:HG12  | 1.85                     | 0.75              |
| 77:3O:47:LEU:CD2   | 77:3O:79:ILE:HG23  | 2.16                     | 0.75              |
| 1:1A:99:A:H2'      | 1:1A:100:C:O2      | 1.85                     | 0.75              |
| 1:1A:4423:U:H3'    | 41:2g:97:ARG:HH21  | 1.51                     | 0.75              |
| 47:2m:146:G:O2'    | 47:2m:147:A:H5'    | 1.87                     | 0.75              |
| 47:2m:674:C:H2'    | 47:2m:675:U:C6     | 2.22                     | 0.75              |
| 47:2m:1266:C:N3    | 47:2m:1517:G:N2    | 2.35                     | 0.75              |
| 48:2n:128:ARG:HA   | 48:2n:131:HIS:CE1  | 2.22                     | 0.75              |
| 62:21:40:ILE:HG22  | 62:21:44:LYS:HZ3   | 1.51                     | 0.75              |
| 76:3N:9:THR:OG1    | 76:3N:23:MET:HE2   | 1.85                     | 0.75              |
| 1:1A:691:C:H2'     | 1:1A:692:A:C8      | 2.22                     | 0.75              |
| 1:1A:1048:G:H2'    | 1:1A:1049:C:C6     | 2.22                     | 0.75              |
| 1:1A:1342:A:O2'    | 1:1A:1343:A:H5'    | 1.87                     | 0.75              |
| 1:1A:1761:G:O6     | 1:1A:1772:C:N4     | 2.19                     | 0.75              |
| 13:2E:38:LYS:O     | 13:2E:42:GLN:HG2   | 1.86                     | 0.75              |
| 47:2m:392:A:O2'    | 47:2m:393:U:H5'    | 1.87                     | 0.75              |
| 53:2s:11:PRO:HD2   | 53:2s:45:ILE:O     | 1.86                     | 0.75              |
| 1:1A:2745:A:H2'    | 1:1A:2746:A:H8     | 1.51                     | 0.75              |
| 46:2l:160:LYS:HG3  | 46:2l:161:LYS:H    | 1.52                     | 0.75              |
| 47:2m:1391:C:H4'   | 67:3E:55:LEU:HD23  | 1.69                     | 0.75              |
| 47:2m:1450:G:H2'   | 47:2m:1451:G:O4'   | 1.86                     | 0.75              |
| 76:3N:27:VAL:HG11  | 76:3N:35:VAL:HG11  | 1.69                     | 0.75              |
| 1:1A:2255:C:H2'    | 1:1A:2255:C:O2     | 1.87                     | 0.75              |
| 1:1A:2506:G:H4'    | 1:1A:2507:A:OP1    | 1.87                     | 0.75              |
| 28:2T:103:ASP:HB3  | 28:2T:106:LEU:HD12 | 1.69                     | 0.75              |
| 47:2m:337:C:C2'    | 47:2m:338:G:H4'    | 2.17                     | 0.75              |
| 47:2m:1671:G:O2'   | 47:2m:1672:U:O5'   | 2.03                     | 0.75              |
| 56:2v:74:SER:O     | 56:2v:90:ARG:NH1   | 2.19                     | 0.75              |
| 60:2z:84:LEU:HD22  | 60:2z:95:TYR:HB3   | 1.67                     | 0.75              |
| 75:3M:35:VAL:O     | 75:3M:39:THR:HG23  | 1.87                     | 0.75              |
| 1:1A:2905:C:O2'    | 1:1A:2907:G:OP1    | 2.04                     | 0.75              |
| 1:1A:4745:G:H22    | 1:1A:4954:G:H1     | 1.35                     | 0.75              |
| 1:1A:4910:G:N2     | 17:2I:106:ASP:O    | 2.20                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:2G:126:GLU:HG3  | 17:2I:185:VAL:HG13 | 1.68                     | 0.75              |
| 46:2I:32:VAL:HG13  | 46:2I:169:VAL:HG22 | 1.67                     | 0.75              |
| 47:2m:112:U:H5''   | 47:2m:113:G:OP1    | 1.87                     | 0.75              |
| 47:2m:912:C:C2     | 47:2m:914:U:H1'    | 2.21                     | 0.75              |
| 47:2m:1042:A:N6    | 47:2m:1074:C:O2    | 2.19                     | 0.75              |
| 52:2r:49:LEU:HD12  | 58:2x:50:LYS:HG3   | 1.68                     | 0.75              |
| 11:2C:12:ILE:HD11  | 11:2C:18:ILE:HD11  | 1.69                     | 0.74              |
| 46:2I:159:MET:SD   | 46:2I:159:MET:N    | 2.60                     | 0.74              |
| 47:2m:472:C:H4'    | 47:2m:474:G:OP1    | 1.87                     | 0.74              |
| 47:2m:1281:G:O2'   | 47:2m:1282:A:H5'   | 1.87                     | 0.74              |
| 47:2m:1622:U:O4    | 57:2w:122:THR:N    | 2.20                     | 0.74              |
| 49:2o:35:ALA:HA    | 49:2o:98:THR:HG22  | 1.67                     | 0.74              |
| 59:2y:41:ILE:HD13  | 59:2y:50:ILE:HD12  | 1.68                     | 0.74              |
| 62:2I:24:LEU:HD11  | 62:2I:87:ARG:CB    | 2.17                     | 0.74              |
| 64:3B:102:VAL:CG1  | 64:3B:120:PHE:HB3  | 2.17                     | 0.74              |
| 71:3I:81:LEU:O     | 71:3I:84:ILE:HG22  | 1.87                     | 0.74              |
| 1:1A:3699:C:O2'    | 1:1A:3775:A:O2'    | 2.04                     | 0.74              |
| 1:1A:3756:A:O2'    | 1:1A:3757:G:H5'    | 1.87                     | 0.74              |
| 1:1A:4526:U:O2'    | 1:1A:4527:G:H5'    | 1.87                     | 0.74              |
| 1:1A:4873:G:H4'    | 1:1A:4874:A:H5'    | 1.69                     | 0.74              |
| 10:2B:128:VAL:O    | 10:2B:130:THR:HG23 | 1.86                     | 0.74              |
| 14:2F:58:ILE:HD13  | 14:2F:157:VAL:HG22 | 1.67                     | 0.74              |
| 47:2m:118:C:H1'    | 47:2m:445:A:C5     | 2.22                     | 0.74              |
| 47:2m:158:A:H2'    | 47:2m:159:A:C1'    | 2.17                     | 0.74              |
| 47:2m:1845:A:H2'   | 47:2m:1846:G:C8    | 2.22                     | 0.74              |
| 48:2n:12:GLU:HB3   | 59:2y:111:PHE:HE2  | 1.50                     | 0.74              |
| 68:3F:258:ILE:HG22 | 68:3F:267:VAL:HB   | 1.68                     | 0.74              |
| 69:3G:142:LYS:HD3  | 69:3G:153:GLY:HA3  | 1.69                     | 0.74              |
| 1:1A:691:C:H2'     | 1:1A:692:A:H8      | 1.51                     | 0.74              |
| 1:1A:3960:A:N7     | 1:1A:3961:G:O2'    | 2.19                     | 0.74              |
| 13:2E:175:LEU:HB3  | 13:2E:176:PRO:HD2  | 1.70                     | 0.74              |
| 50:2p:121:GLY:HA2  | 50:2p:124:ARG:HE   | 1.51                     | 0.74              |
| 1:1A:1274:A:O2'    | 1:1A:1275:G:H5'    | 1.87                     | 0.74              |
| 1:1A:3599:A:H2'    | 1:1A:3600:G:C8     | 2.23                     | 0.74              |
| 1:1A:4900:C:OP1    | 1:1A:4900:C:H3'    | 1.88                     | 0.74              |
| 36:2b:87:LYS:N     | 38:2d:80:GLU:OE2   | 2.19                     | 0.74              |
| 1:1A:1857:C:H2'    | 1:1A:1858:A:H8     | 1.53                     | 0.74              |
| 1:1A:4541:G:N2     | 1:1A:4544:A:OP2    | 2.15                     | 0.74              |
| 34:2Z:106:TYR:HB2  | 34:2Z:107:PRO:HD3  | 1.69                     | 0.74              |
| 47:2m:980:A:H2'    | 47:2m:981:A:H8     | 1.52                     | 0.74              |
| 50:2p:227:LYS:HE2  | 68:3F:184:LEU:HD23 | 1.69                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:2R:37:LYS:O     | 26:2R:39:LYS:N     | 2.20                     | 0.74              |
| 28:2T:30:ASP:OD1   | 28:2T:77:TYR:OH    | 2.03                     | 0.74              |
| 52:2r:102:LEU:HD11 | 77:3O:108:ILE:HG21 | 1.70                     | 0.74              |
| 57:2w:83:MET:HG3   | 57:2w:116:LEU:CD2  | 2.16                     | 0.74              |
| 77:3O:46:ASN:HB2   | 77:3O:78:LYS:O     | 1.88                     | 0.74              |
| 1:1A:136:C:H4'     | 1:1A:137:G:C8      | 2.22                     | 0.74              |
| 1:1A:666:G:O2'     | 1:1A:667:A:H3'     | 1.88                     | 0.74              |
| 1:1A:4323:A:C2     | 7:1G:146:LEU:HD23  | 2.23                     | 0.74              |
| 11:2C:18:ILE:CG2   | 11:2C:27:VAL:HG22  | 2.18                     | 0.74              |
| 43:2i:14:LYS:HE2   | 43:2i:77:CYS:HB2   | 1.70                     | 0.74              |
| 47:2m:1528:G:O2'   | 47:2m:1666:C:OP1   | 2.06                     | 0.74              |
| 58:2x:97:GLN:HB2   | 58:2x:105:LYS:CD   | 2.17                     | 0.74              |
| 77:3O:64:ASN:O     | 77:3O:111:ARG:NE   | 2.21                     | 0.74              |
| 1:1A:130:C:H2'     | 1:1A:131:C:C1'     | 2.17                     | 0.74              |
| 1:1A:1591:U:OP2    | 1:1A:2856:C:O2'    | 2.04                     | 0.74              |
| 1:1A:4751:G:H2'    | 1:1A:4752:U:H5'    | 1.70                     | 0.74              |
| 46:2l:30:GLU:OE2   | 46:2l:212:LYS:NZ   | 2.15                     | 0.74              |
| 47:2m:215:G:O2'    | 47:2m:216:C:H5''   | 1.88                     | 0.74              |
| 47:2m:570:C:O2'    | 76:3N:34:THR:O     | 2.05                     | 0.74              |
| 47:2m:1412:C:H5'   | 47:2m:1413:G:OP2   | 1.88                     | 0.74              |
| 56:2v:91:ASP:N     | 56:2v:91:ASP:OD1   | 2.20                     | 0.74              |
| 1:1A:138:G:O2'     | 1:1A:139:G:H5'     | 1.88                     | 0.74              |
| 1:1A:2481:G:H2'    | 1:1A:2482:C:C6     | 2.23                     | 0.74              |
| 1:1A:3706:C:OP2    | 81:1A:5116:84D:N   | 2.20                     | 0.74              |
| 1:1A:4598:C:OP2    | 1:1A:4599:A:O2'    | 2.02                     | 0.74              |
| 7:1G:126:THR:HG22  | 7:1G:128:ASP:H     | 1.52                     | 0.74              |
| 11:2C:107:GLU:OE1  | 11:2C:107:GLU:N    | 2.21                     | 0.74              |
| 12:2D:76:MET:HE3   | 12:2D:138:ILE:HG21 | 1.70                     | 0.74              |
| 14:2F:80:GLU:HG2   | 14:2F:110:LEU:HD12 | 1.68                     | 0.74              |
| 27:2S:47:MET:HE1   | 27:2S:118:ILE:CG2  | 2.17                     | 0.74              |
| 47:2m:1285:G:O2'   | 47:2m:1286:G:H5'   | 1.87                     | 0.74              |
| 50:2p:101:GLN:HG3  | 50:2p:126:ILE:CD1  | 2.14                     | 0.74              |
| 53:2s:130:LEU:HD13 | 53:2s:177:TYR:CE1  | 2.23                     | 0.74              |
| 53:2s:163:GLN:O    | 53:2s:167:GLU:HB2  | 1.88                     | 0.74              |
| 62:21:28:ASN:ND2   | 62:21:31:SER:OG    | 2.20                     | 0.74              |
| 1:1A:106:A:H1'     | 1:1A:336:A:C8      | 2.23                     | 0.74              |
| 1:1A:1095:A:H2'    | 1:1A:1096:C:H6     | 1.51                     | 0.74              |
| 1:1A:4426:C:H2'    | 1:1A:4427:G:H5'    | 1.68                     | 0.74              |
| 2:1B:52:C:H4'      | 13:2E:11:PRO:HB2   | 1.68                     | 0.74              |
| 7:1G:223:PHE:HB3   | 7:1G:226:TYR:HB2   | 1.69                     | 0.74              |
| 14:2F:63:THR:HG22  | 14:2F:65:ARG:H     | 1.53                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:2J:85:LYS:O     | 18:2J:89:GLU:HG2   | 1.88                     | 0.74              |
| 49:2o:196:ASP:HA   | 49:2o:199:LYS:CE   | 2.17                     | 0.74              |
| 70:3H:42:GLY:HA3   | 70:3H:45:TRP:CE3   | 2.23                     | 0.74              |
| 26:2R:153:ILE:HG22 | 26:2R:155:ILE:HG23 | 1.70                     | 0.73              |
| 46:2l:31:THR:O     | 46:2l:208:SER:OG   | 2.00                     | 0.73              |
| 46:2l:95:LYS:HB3   | 46:2l:104:ALA:HB1  | 1.70                     | 0.73              |
| 47:2m:23:G:O2'     | 47:2m:24:C:H5'     | 1.88                     | 0.73              |
| 47:2m:51:U:H2'     | 47:2m:52:G:H8      | 1.52                     | 0.73              |
| 47:2m:189:U:H1'    | 47:2m:211:G:N2     | 2.02                     | 0.73              |
| 47:2m:878:G:H5'    | 47:2m:879:C:C5     | 2.23                     | 0.73              |
| 47:2m:888:U:O2'    | 47:2m:890:U:OP1    | 2.06                     | 0.73              |
| 47:2m:1228:A:H2'   | 47:2m:1229:G:H8    | 1.53                     | 0.73              |
| 51:2q:185:GLY:H    | 51:2q:189:LEU:HD13 | 1.53                     | 0.73              |
| 60:2z:80:PRO:HG2   | 60:2z:83:PHE:CD2   | 2.23                     | 0.73              |
| 62:21:24:LEU:CD1   | 62:21:87:ARG:HB2   | 2.17                     | 0.73              |
| 77:3O:62:VAL:HG22  | 77:3O:63:PRO:HD3   | 1.70                     | 0.73              |
| 1:1A:2431:A:OP1    | 40:2f:41:ARG:NH1   | 2.20                     | 0.73              |
| 21:2M:164:LYS:HB3  | 21:2M:165:PRO:CD   | 2.18                     | 0.73              |
| 50:2p:120:TYR:OH   | 69:3G:146:GLU:HG3  | 1.88                     | 0.73              |
| 77:3O:102:LYS:O    | 77:3O:102:LYS:HG2  | 1.86                     | 0.73              |
| 1:1A:132:G:N7      | 1:1A:133:C:O2'     | 2.19                     | 0.73              |
| 1:1A:319:A:H1'     | 1:1A:3726:A:C8     | 2.21                     | 0.73              |
| 1:1A:1633:G:H5'    | 1:1A:1634:A:OP1    | 1.87                     | 0.73              |
| 1:1A:1669:A:H4'    | 1:1A:1685:G:H22    | 1.53                     | 0.73              |
| 1:1A:3641:U:OP2    | 1:1A:3646:A:N6     | 2.19                     | 0.73              |
| 1:1A:4594:U:H2'    | 1:1A:4595:G:C8     | 2.23                     | 0.73              |
| 5:1E:199:GLU:OE2   | 5:1E:200:ARG:NH1   | 2.22                     | 0.73              |
| 47:2m:30:C:OP1     | 64:3B:138:LYS:NZ   | 2.17                     | 0.73              |
| 47:2m:1347:U:H2'   | 47:2m:1348:G:C8    | 2.22                     | 0.73              |
| 52:2r:112:LEU:HD13 | 52:2r:177:LEU:HD11 | 1.70                     | 0.73              |
| 1:1A:1503:A:H4'    | 1:1A:1504:G:H5'    | 1.70                     | 0.73              |
| 1:1A:3717:A:OP2    | 1:1A:3735:G:N2     | 2.20                     | 0.73              |
| 1:1A:4504:C:H2'    | 1:1A:4505:C:C6     | 2.22                     | 0.73              |
| 4:1D:234:LYS:HG3   | 4:1D:234:LYS:O     | 1.89                     | 0.73              |
| 5:1E:71:GLU:OE1    | 25:2Q:1:MET:N      | 2.16                     | 0.73              |
| 47:2m:566:U:H3'    | 47:2m:567:C:H6     | 1.53                     | 0.73              |
| 47:2m:889:U:H5''   | 47:2m:890:U:H5'    | 1.70                     | 0.73              |
| 47:2m:957:A:O2'    | 47:2m:958:G:O5'    | 2.05                     | 0.73              |
| 47:2m:1568:C:H5''  | 61:20:96:SER:HB2   | 1.70                     | 0.73              |
| 47:2m:1845:A:H2'   | 47:2m:1846:G:H8    | 1.52                     | 0.73              |
| 58:2x:32:ILE:HD12  | 58:2x:68:ILE:HG13  | 1.69                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 60:2z:23:ARG:HB3  | 77:3O:48:VAL:HG11  | 1.68                     | 0.73              |
| 72:3J:48:HIS:HB2  | 72:3J:111:VAL:HG23 | 1.71                     | 0.73              |
| 1:1A:127:G:H2'    | 1:1A:128:C:H5'     | 1.69                     | 0.73              |
| 1:1A:2833:A:O2'   | 1:1A:2834:C:H5'    | 1.87                     | 0.73              |
| 1:1A:4580:U:O2'   | 5:1E:182:GLU:OE2   | 2.04                     | 0.73              |
| 31:2W:28:VAL:HG11 | 31:2W:33:GLN:HB3   | 1.69                     | 0.73              |
| 47:2m:396:U:OP2   | 56:2v:79:LYS:NZ    | 2.17                     | 0.73              |
| 53:2s:144:ILE:H   | 53:2s:144:ILE:HD12 | 1.53                     | 0.73              |
| 59:2y:34:VAL:O    | 59:2y:38:ILE:HG13  | 1.89                     | 0.73              |
| 66:3D:14:VAL:HG23 | 66:3D:32:VAL:HG12  | 1.67                     | 0.73              |
| 1:1A:179:G:O2'    | 1:1A:180:C:OP1     | 2.07                     | 0.73              |
| 13:2E:57:VAL:HG23 | 13:2E:59:SER:H     | 1.54                     | 0.73              |
| 48:2n:37:TYR:CD2  | 48:2n:162:PRO:HG3  | 2.23                     | 0.73              |
| 68:3F:208:ALA:HB2 | 68:3F:218:LEU:HG   | 1.70                     | 0.73              |
| 77:3O:77:LEU:HD12 | 77:3O:78:LYS:H     | 1.53                     | 0.73              |
| 1:1A:1602:U:OP1   | 38:2d:2:THR:OG1    | 2.05                     | 0.73              |
| 47:2m:945:U:H2'   | 47:2m:946:U:C6     | 2.22                     | 0.73              |
| 47:2m:963:A:H2'   | 47:2m:964:A:C8     | 2.23                     | 0.73              |
| 47:2m:1245:G:O2'  | 47:2m:1492:U:OP1   | 2.06                     | 0.73              |
| 47:2m:1259:A:N6   | 47:2m:1518:C:O2    | 2.22                     | 0.73              |
| 55:2u:86:PRO:HB2  | 55:2u:88:GLU:OE1   | 1.88                     | 0.73              |
| 4:1D:30:ARG:NH1   | 4:1D:36:GLU:OE1    | 2.19                     | 0.73              |
| 4:1D:245:ARG:NH1  | 4:1D:245:ARG:O     | 2.21                     | 0.73              |
| 11:2C:105:ILE:CG2 | 11:2C:109:GLY:HA2  | 2.19                     | 0.73              |
| 46:2l:23:ARG:NH2  | 46:2l:174:MET:O    | 2.22                     | 0.73              |
| 47:2m:616:A:N3    | 79:3Q:12:VAL:HG21  | 2.03                     | 0.73              |
| 53:2s:148:LEU:O   | 53:2s:148:LEU:HD13 | 1.87                     | 0.73              |
| 62:21:24:LEU:HD12 | 62:21:24:LEU:O     | 1.88                     | 0.73              |
| 68:3F:285:GLN:O   | 68:3F:303:THR:N    | 2.16                     | 0.73              |
| 78:3P:33:MET:HE3  | 78:3P:79:PHE:HD1   | 1.54                     | 0.73              |
| 1:1A:383:A:O2'    | 1:1A:384:A:O5'     | 2.05                     | 0.73              |
| 1:1A:2107:C:N4    | 1:1A:2108:G:O6     | 2.20                     | 0.73              |
| 1:1A:4099:G:H4'   | 1:1A:4111:U:O2     | 1.87                     | 0.73              |
| 1:1A:4109:G:O2'   | 1:1A:4110:C:O4'    | 2.05                     | 0.73              |
| 5:1E:189:THR:O    | 5:1E:193:LYS:HG2   | 1.87                     | 0.73              |
| 40:2f:9:ILE:CD1   | 40:2f:51:LEU:HD11  | 2.19                     | 0.73              |
| 49:2o:168:MET:HG2 | 49:2o:197:ILE:HG21 | 1.70                     | 0.73              |
| 57:2w:108:LYS:HD3 | 57:2w:110:GLU:H    | 1.53                     | 0.73              |
| 59:2y:17:ILE:HD12 | 59:2y:58:MET:CE    | 2.19                     | 0.73              |
| 1:1A:2256:C:H2'   | 1:1A:2257:C:H6     | 1.53                     | 0.73              |
| 1:1A:4096:C:N4    | 1:1A:4113:U:O2'    | 2.22                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4251:A:H1'    | 13:2E:110:GLN:OE1  | 1.88                     | 0.73              |
| 1:1A:4462:C:O2'    | 1:1A:4463:U:H5'    | 1.89                     | 0.73              |
| 27:2S:82:ILE:CD1   | 27:2S:99:ILE:HD11  | 2.19                     | 0.73              |
| 47:2m:1447:G:O2'   | 62:21:33:GLU:OE1   | 2.07                     | 0.73              |
| 48:2n:19:LEU:HB3   | 59:2y:96:ILE:HG21  | 1.69                     | 0.73              |
| 48:2n:145:ILE:HG12 | 48:2n:159:ILE:CD1  | 2.19                     | 0.73              |
| 49:2o:38:MET:HE2   | 49:2o:185:VAL:HG11 | 1.71                     | 0.73              |
| 50:2p:12:VAL:O     | 50:2p:16:ILE:HG23  | 1.89                     | 0.73              |
| 1:1A:418:A:OP2     | 3:1C:16:G:N2       | 2.21                     | 0.72              |
| 1:1A:1759:G:H1     | 1:1A:1773:U:H3     | 1.37                     | 0.72              |
| 1:1A:4104:G:H2'    | 1:1A:4106:G:N2     | 2.03                     | 0.72              |
| 12:2D:144:ASN:O    | 12:2D:148:VAL:HG13 | 1.88                     | 0.72              |
| 34:2Z:45:LYS:HD2   | 34:2Z:105:LEU:HA   | 1.70                     | 0.72              |
| 47:2m:1449:G:O2'   | 47:2m:1450:G:H5'   | 1.89                     | 0.72              |
| 47:2m:1643:U:HO2'  | 47:2m:1644:C:H6    | 1.37                     | 0.72              |
| 52:2r:175:ASP:HA   | 52:2r:178:ILE:HD11 | 1.71                     | 0.72              |
| 53:2s:111:LYS:HD3  | 53:2s:112:ASN:H    | 1.53                     | 0.72              |
| 72:3J:97:GLU:N     | 72:3J:97:GLU:OE1   | 2.22                     | 0.72              |
| 1:1A:1082:C:H1'    | 1:1A:1083:U:C6     | 2.24                     | 0.72              |
| 1:1A:1202:C:H3'    | 1:1A:1203:G:C5'    | 2.19                     | 0.72              |
| 10:2B:243:GLY:O    | 10:2B:247:VAL:HG13 | 1.90                     | 0.72              |
| 47:2m:1823:A:O2'   | 47:2m:1824:A:H5'   | 1.88                     | 0.72              |
| 57:2w:57:LEU:HG    | 57:2w:89:MET:CE    | 2.19                     | 0.72              |
| 57:2w:80:LEU:HD23  | 57:2w:80:LEU:H     | 1.54                     | 0.72              |
| 58:2x:43:GLU:HB3   | 58:2x:44:PRO:CD    | 2.18                     | 0.72              |
| 59:2y:16:ILE:HG22  | 59:2y:17:ILE:HD13  | 1.69                     | 0.72              |
| 71:3I:82:VAL:HG21  | 71:3I:92:MET:CE    | 2.19                     | 0.72              |
| 1:1A:2580:U:O2'    | 28:2T:79:HIS:ND1   | 2.22                     | 0.72              |
| 1:1A:2903:G:H4'    | 1:1A:3591:C:N4     | 2.03                     | 0.72              |
| 1:1A:3671:G:H2'    | 1:1A:3672:G:C8     | 2.23                     | 0.72              |
| 1:1A:3689:G:O2'    | 1:1A:3818:U:OP2    | 2.07                     | 0.72              |
| 1:1A:4103:C:O2'    | 1:1A:4104:G:H5''   | 1.89                     | 0.72              |
| 5:1E:224:LYS:HG2   | 5:1E:340:THR:CG2   | 2.20                     | 0.72              |
| 10:2B:107:LYS:HG2  | 10:2B:108:GLN:OE1  | 1.89                     | 0.72              |
| 47:2m:1119:A:H2'   | 47:2m:1120:U:C6    | 2.24                     | 0.72              |
| 58:2x:55:VAL:HA    | 58:2x:63:PHE:CE2   | 2.25                     | 0.72              |
| 1:1A:279:A:O2'     | 1:1A:280:G:OP2     | 2.06                     | 0.72              |
| 1:1A:2489:C:H4'    | 1:1A:2491:C:N3     | 2.05                     | 0.72              |
| 1:1A:3664:G:H2'    | 1:1A:3665:G:H8     | 1.53                     | 0.72              |
| 9:2A:52:GLU:HG3    | 30:2V:96:LEU:CD1   | 2.20                     | 0.72              |
| 11:2C:8:GLN:HG2    | 11:2C:74:CYS:SG    | 2.30                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:2T:89:ILE:CD1   | 28:2T:91:LEU:HD13  | 2.19                     | 0.72              |
| 36:2b:103:LYS:NZ   | 36:2b:111:GLU:OE1  | 2.18                     | 0.72              |
| 47:2m:26:U:H2'     | 47:2m:27:A:C8      | 2.24                     | 0.72              |
| 47:2m:921:G:C2     | 78:3P:22:LYS:HG2   | 2.24                     | 0.72              |
| 51:2q:100:ARG:HB2  | 51:2q:114:ILE:HD13 | 1.71                     | 0.72              |
| 58:2x:54:PRO:HG2   | 58:2x:88:ILE:HD11  | 1.71                     | 0.72              |
| 59:2y:60:ARG:HG2   | 59:2y:66:VAL:HG11  | 1.69                     | 0.72              |
| 70:3H:199:THR:HG22 | 70:3H:203:LYS:CE   | 2.18                     | 0.72              |
| 78:3P:81:ARG:NE    | 78:3P:84:HIS:O     | 2.22                     | 0.72              |
| 46:2l:59:PRO:HB3   | 46:2l:170:GLY:HA3  | 1.71                     | 0.72              |
| 47:2m:614:C:H4'    | 47:2m:615:C:O5'    | 1.89                     | 0.72              |
| 47:2m:901:G:N2     | 47:2m:902:G:H1'    | 2.05                     | 0.72              |
| 50:2p:5:ILE:CG2    | 50:2p:10:LYS:HD2   | 2.19                     | 0.72              |
| 51:2q:55:ALA:CB    | 51:2q:61:VAL:HG22  | 2.20                     | 0.72              |
| 54:2t:100:CYS:SG   | 54:2t:175:ILE:HG13 | 2.30                     | 0.72              |
| 58:2x:93:VAL:HG11  | 58:2x:109:LYS:NZ   | 2.05                     | 0.72              |
| 79:3Q:8:ARG:HG3    | 79:3Q:8:ARG:O      | 1.89                     | 0.72              |
| 1:1A:3736:A:H2'    | 1:1A:3737:A:C8     | 2.24                     | 0.72              |
| 2:1B:58:A:H2'      | 2:1B:59:G:H8       | 1.52                     | 0.72              |
| 6:1F:65:GLU:O      | 6:1F:78:ARG:N      | 2.19                     | 0.72              |
| 47:2m:889:U:C5'    | 47:2m:890:U:H5'    | 2.19                     | 0.72              |
| 47:2m:1839:U:H2'   | 47:2m:1840:U:C6    | 2.24                     | 0.72              |
| 48:2n:126:ASP:OD1  | 48:2n:129:ALA:N    | 2.17                     | 0.72              |
| 54:2t:114:GLU:OE2  | 54:2t:120:PRO:HA   | 1.89                     | 0.72              |
| 55:2u:85:LEU:HD21  | 55:2u:89:ILE:HB    | 1.71                     | 0.72              |
| 69:3G:165:VAL:HG21 | 69:3G:217:ALA:HB1  | 1.69                     | 0.72              |
| 1:1A:1830:G:O2'    | 1:1A:1831:G:H5'    | 1.90                     | 0.72              |
| 1:1A:3773:U:H4'    | 1:1A:3774:A:O5'    | 1.90                     | 0.72              |
| 1:1A:3975:C:H2'    | 1:1A:3976:C:C4     | 2.25                     | 0.72              |
| 46:2l:54:ARG:NH1   | 46:2l:148:VAL:O    | 2.23                     | 0.72              |
| 65:3C:47:ALA:HA    | 65:3C:50:VAL:HG23  | 1.71                     | 0.72              |
| 23:2O:36:ALA:O     | 23:2O:40:GLU:HG3   | 1.89                     | 0.72              |
| 46:2l:54:ARG:HD2   | 46:2l:152:LYS:HB3  | 1.72                     | 0.72              |
| 46:2l:142:GLU:HG2  | 46:2l:144:MET:HB2  | 1.71                     | 0.72              |
| 47:2m:1408:U:O2'   | 58:2x:71:ARG:NH1   | 2.22                     | 0.72              |
| 47:2m:1419:C:OP2   | 61:20:125:PRO:HB3  | 1.90                     | 0.72              |
| 50:2p:54:ARG:HG2   | 50:2p:57:ASN:HB2   | 1.71                     | 0.72              |
| 50:2p:167:TYR:OH   | 50:2p:203:PRO:HA   | 1.89                     | 0.72              |
| 62:21:35:VAL:CG2   | 62:21:107:GLU:HG2  | 2.18                     | 0.72              |
| 72:3J:25:ALA:HB1   | 72:3J:31:LEU:HD11  | 1.70                     | 0.72              |
| 1:1A:972:C:C6      | 8:1H:126:LEU:HD13  | 2.23                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1763:C:C2'    | 1:1A:1764:G:H5'    | 2.20                     | 0.72              |
| 1:1A:2647:A:H62    | 1:1A:2686:G:H8     | 1.35                     | 0.72              |
| 1:1A:2702:C:OP1    | 23:2O:101:ARG:NH2  | 2.18                     | 0.72              |
| 6:1F:109:ARG:O     | 6:1F:109:ARG:HG2   | 1.90                     | 0.72              |
| 47:2m:840:C:H5'    | 47:2m:841:G:H5''   | 1.72                     | 0.72              |
| 47:2m:1007:C:H2'   | 47:2m:1008:A:C8    | 2.24                     | 0.72              |
| 47:2m:1088:U:H4'   | 47:2m:1089:G:OP2   | 1.88                     | 0.72              |
| 47:2m:1249:C:OP2   | 47:2m:1250:A:O2'   | 2.07                     | 0.72              |
| 51:2q:114:ILE:HD12 | 51:2q:118:GLU:OE1  | 1.90                     | 0.72              |
| 54:2t:110:ARG:O    | 54:2t:114:GLU:HG2  | 1.90                     | 0.72              |
| 54:2t:172:LEU:HD12 | 54:2t:172:LEU:O    | 1.90                     | 0.72              |
| 65:3C:44:ILE:HD13  | 65:3C:67:LEU:HD13  | 1.71                     | 0.72              |
| 66:3D:17:VAL:HG12  | 66:3D:19:GLY:H     | 1.55                     | 0.72              |
| 66:3D:45:ASN:ND2   | 66:3D:64:GLU:OE2   | 2.23                     | 0.72              |
| 68:3F:120:ILE:CG2  | 68:3F:132:TRP:HB2  | 2.20                     | 0.72              |
| 76:3N:117:VAL:HG21 | 76:3N:125:VAL:HG21 | 1.72                     | 0.72              |
| 1:1A:1079:C:H2'    | 1:1A:1080:C:C6     | 2.25                     | 0.72              |
| 1:1A:2536:A:H5'    | 39:2e:42:LEU:HD22  | 1.71                     | 0.72              |
| 1:1A:4239:A:H2'    | 1:1A:4240:G:H8     | 1.53                     | 0.72              |
| 23:2O:43:LEU:O     | 23:2O:47:ILE:HG13  | 1.89                     | 0.72              |
| 47:2m:560:A:H5'    | 47:2m:561:A:OP2    | 1.89                     | 0.72              |
| 47:2m:1373:C:OP1   | 59:2y:7:LYS:N      | 2.20                     | 0.72              |
| 47:2m:1513:C:H2'   | 47:2m:1514:G:C8    | 2.24                     | 0.72              |
| 47:2m:1534:C:H5''  | 47:2m:1536:G:H1'   | 1.71                     | 0.72              |
| 47:2m:1679:A:H2'   | 52:2r:60:ARG:HD2   | 1.72                     | 0.72              |
| 52:2r:100:ILE:HD12 | 52:2r:178:ILE:CG2  | 2.19                     | 0.72              |
| 68:3F:52:TYR:CD2   | 68:3F:309:VAL:HG21 | 2.25                     | 0.72              |
| 74:3L:43:HIS:CD2   | 74:3L:55:ARG:HB2   | 2.25                     | 0.72              |
| 1:1A:1656:U:OP2    | 29:2U:26:ARG:NH2   | 2.23                     | 0.71              |
| 1:1A:4993:G:O6     | 1:1A:5058:A:N1     | 2.22                     | 0.71              |
| 47:2m:1623:A:H3'   | 47:2m:1623:A:N3    | 2.05                     | 0.71              |
| 51:2q:56:LEU:N     | 51:2q:60:GLU:OE2   | 2.18                     | 0.71              |
| 53:2s:15:LYS:O     | 53:2s:15:LYS:NZ    | 2.16                     | 0.71              |
| 58:2x:50:LYS:O     | 58:2x:53:GLU:HG3   | 1.90                     | 0.71              |
| 77:3O:57:LYS:HE2   | 77:3O:77:LEU:CD2   | 2.20                     | 0.71              |
| 1:1A:1617:G:H1'    | 1:1A:2513:A:N6     | 2.05                     | 0.71              |
| 8:1H:99:ASP:OD1    | 8:1H:100:LYS:N     | 2.23                     | 0.71              |
| 21:2M:16:CYS:SG    | 21:2M:54:MET:HG3   | 2.29                     | 0.71              |
| 47:2m:51:U:H2'     | 47:2m:52:G:C8      | 2.25                     | 0.71              |
| 50:2p:65:ARG:HA    | 50:2p:68:GLU:OE2   | 1.90                     | 0.71              |
| 60:2z:28:PHE:HE2   | 60:2z:38:ARG:HE    | 1.37                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:3C:25:ASN:ND2   | 65:3C:77:CYS:SG    | 2.60                     | 0.71              |
| 68:3F:116:ASP:HB3  | 68:3F:118:ARG:HD2  | 1.72                     | 0.71              |
| 70:3H:49:VAL:CG2   | 70:3H:115:LYS:HB3  | 2.20                     | 0.71              |
| 1:1A:438:G:O2'     | 1:1A:439:G:H5'     | 1.90                     | 0.71              |
| 1:1A:1378:C:N4     | 14:2F:159:ASN:O    | 2.23                     | 0.71              |
| 8:1H:47:ASN:HB2    | 8:1H:62:MET:HE2    | 1.71                     | 0.71              |
| 13:2E:141:ILE:HA   | 13:2E:144:LYS:HG2  | 1.72                     | 0.71              |
| 25:2Q:101:ARG:HB2  | 25:2Q:105:ARG:NE   | 2.05                     | 0.71              |
| 59:2y:24:LEU:HD11  | 59:2y:58:MET:CE    | 2.18                     | 0.71              |
| 76:3N:60:PHE:CD1   | 76:3N:71:GLY:HA3   | 2.25                     | 0.71              |
| 1:1A:964:A:H2'     | 1:1A:965:G:H4'     | 1.71                     | 0.71              |
| 1:1A:1942:A:H2'    | 1:1A:1943:A:H8     | 1.54                     | 0.71              |
| 5:1E:222:VAL:O     | 5:1E:343:ARG:NH1   | 2.24                     | 0.71              |
| 11:2C:129:ARG:NE   | 11:2C:156:ASN:OD1  | 2.23                     | 0.71              |
| 13:2E:90:ARG:O     | 13:2E:91:GLU:HG3   | 1.91                     | 0.71              |
| 35:2a:107:LEU:HA   | 35:2a:110:GLN:HE21 | 1.56                     | 0.71              |
| 47:2m:74:G:O2'     | 47:2m:75:G:H4'     | 1.90                     | 0.71              |
| 59:2y:56:HIS:HA    | 59:2y:59:LYS:HD3   | 1.73                     | 0.71              |
| 64:3B:61:GLN:HB3   | 64:3B:62:PRO:HD3   | 1.71                     | 0.71              |
| 68:3F:236:ILE:HD11 | 68:3F:250:ALA:HB1  | 1.72                     | 0.71              |
| 70:3H:216:ARG:HH22 | 70:3H:219:GLU:HB3  | 1.55                     | 0.71              |
| 1:1A:468:U:O2'     | 1:1A:469:C:H5'     | 1.90                     | 0.71              |
| 1:1A:3974:G:O6     | 1:1A:4037:C:N4     | 2.24                     | 0.71              |
| 9:2A:182:TYR:CD1   | 9:2A:200:ARG:HD2   | 2.25                     | 0.71              |
| 14:2F:211:LYS:NZ   | 46:2l:180:VAL:O    | 2.19                     | 0.71              |
| 44:2j:28:LYS:O     | 44:2j:28:LYS:HD3   | 1.91                     | 0.71              |
| 47:2m:329:G:H2'    | 47:2m:330:G:C8     | 2.25                     | 0.71              |
| 47:2m:1533:A:H62   | 47:2m:1602:U:H3    | 1.36                     | 0.71              |
| 47:2m:1551:U:O2'   | 47:2m:1553:C:OP1   | 2.09                     | 0.71              |
| 51:2q:66:MET:HA    | 51:2q:66:MET:HE3   | 1.72                     | 0.71              |
| 57:2w:75:VAL:HA    | 57:2w:93:MET:HG3   | 1.73                     | 0.71              |
| 58:2x:111:ILE:O    | 58:2x:114:GLN:HG3  | 1.90                     | 0.71              |
| 59:2y:74:GLN:HA    | 59:2y:77:GLU:OE2   | 1.90                     | 0.71              |
| 70:3H:137:ARG:O    | 70:3H:141:ILE:HG13 | 1.90                     | 0.71              |
| 77:3O:62:VAL:HA    | 77:3O:65:TYR:CE2   | 2.25                     | 0.71              |
| 1:1A:2098:G:O2'    | 1:1A:2099:G:O5'    | 2.07                     | 0.71              |
| 1:1A:3634:G:N2     | 1:1A:3636:C:H5''   | 2.06                     | 0.71              |
| 1:1A:3877:A:N3     | 1:1A:4401:G:O2'    | 2.18                     | 0.71              |
| 1:1A:4060:U:O2'    | 1:1A:4061:G:O5'    | 2.08                     | 0.71              |
| 36:2b:91:MET:O     | 36:2b:94:ARG:HG2   | 1.90                     | 0.71              |
| 46:2l:17:VAL:HG12  | 46:2l:19:HIS:CD2   | 2.25                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:2l:106:LYS:HD2  | 46:2l:107:TYR:HB2  | 1.71                     | 0.71              |
| 47:2m:12:U:H2'     | 47:2m:13:C:C6      | 2.25                     | 0.71              |
| 47:2m:1364:U:O4    | 47:2m:1375:G:N2    | 2.17                     | 0.71              |
| 50:2p:214:LYS:HG3  | 50:2p:215:ASP:H    | 1.55                     | 0.71              |
| 52:2r:193:LYS:O    | 52:2r:197:GLU:HG2  | 1.90                     | 0.71              |
| 68:3F:236:ILE:CD1  | 68:3F:250:ALA:HB1  | 2.20                     | 0.71              |
| 1:1A:1433:A:N6     | 1:1A:1451:G:O2'    | 2.24                     | 0.71              |
| 1:1A:2789:A:HO2'   | 40:2f:45:ARG:HH22  | 1.34                     | 0.71              |
| 1:1A:4112:C:H2'    | 1:1A:4113:U:H5'    | 1.73                     | 0.71              |
| 2:1B:31:G:O2'      | 2:1B:32:A:H5'      | 1.90                     | 0.71              |
| 5:1E:153:MET:CG    | 5:1E:194:LEU:HD11  | 2.20                     | 0.71              |
| 11:2C:4:ILE:HG12   | 11:2C:61:TRP:CH2   | 2.26                     | 0.71              |
| 14:2F:145:LYS:HE2  | 14:2F:145:LYS:HA   | 1.71                     | 0.71              |
| 23:2O:72:VAL:O     | 23:2O:72:VAL:HG12  | 1.88                     | 0.71              |
| 47:2m:26:U:H2'     | 47:2m:27:A:H8      | 1.56                     | 0.71              |
| 47:2m:1136:U:H2'   | 47:2m:1137:U:C6    | 2.26                     | 0.71              |
| 47:2m:1262:C:H5''  | 47:2m:1263:U:C5    | 2.26                     | 0.71              |
| 48:2n:85:ARG:HG3   | 48:2n:89:LYS:CE    | 2.20                     | 0.71              |
| 52:2r:20:PHE:HZ    | 52:2r:94:LYS:HD3   | 1.56                     | 0.71              |
| 64:3B:10:ALA:O     | 64:3B:14:ARG:HG2   | 1.91                     | 0.71              |
| 75:3M:76:SER:OG    | 75:3M:77:PRO:HD3   | 1.90                     | 0.71              |
| 76:3N:10:ARG:NH1   | 76:3N:26:ASP:OD1   | 2.22                     | 0.71              |
| 1:1A:739:G:O2'     | 1:1A:740:G:H5''    | 1.90                     | 0.71              |
| 1:1A:2260:C:OP1    | 8:1H:108:LYS:NZ    | 2.18                     | 0.71              |
| 1:1A:3732:A:H2'    | 1:1A:3733:A:H8     | 1.56                     | 0.71              |
| 1:1A:3765:G:N2     | 47:2m:1828:C:O4'   | 2.23                     | 0.71              |
| 23:2O:38:ASN:O     | 23:2O:41:GLN:HG3   | 1.89                     | 0.71              |
| 47:2m:126:G:O6     | 70:3H:196:LYS:NZ   | 2.22                     | 0.71              |
| 47:2m:955:A:N6     | 47:2m:971:G:O2'    | 2.22                     | 0.71              |
| 50:2p:164:VAL:HG23 | 50:2p:164:VAL:O    | 1.88                     | 0.71              |
| 56:2v:4:ILE:HD12   | 56:2v:56:ILE:HD12  | 1.73                     | 0.71              |
| 77:3O:99:LEU:HD21  | 77:3O:102:LYS:CB   | 2.11                     | 0.71              |
| 1:1A:730:G:OP2     | 9:2A:76:ARG:NE     | 2.24                     | 0.71              |
| 1:1A:1628:C:OP2    | 4:1D:9:ARG:HD2     | 1.91                     | 0.71              |
| 1:1A:2781:G:O2'    | 1:1A:2782:U:H5'    | 1.91                     | 0.71              |
| 1:1A:3710:G:H4'    | 1:1A:3711:A:O5'    | 1.91                     | 0.71              |
| 1:1A:3755:G:H1     | 1:1A:3768:U:H3     | 1.37                     | 0.71              |
| 1:1A:4537:C:H2'    | 1:1A:4538:G:H8     | 1.54                     | 0.71              |
| 10:2B:257:LYS:O    | 10:2B:261:LEU:HD23 | 1.91                     | 0.71              |
| 14:2F:139:SER:N    | 14:2F:142:GLU:OE2  | 2.23                     | 0.71              |
| 21:2M:99:ASP:OD2   | 21:2M:108:GLN:NE2  | 2.24                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:291:G:N2    | 47:2m:293:C:OP2    | 2.22                     | 0.71              |
| 47:2m:558:G:N3    | 47:2m:559:G:N2     | 2.34                     | 0.71              |
| 47:2m:639:C:H2'   | 47:2m:640:A:C8     | 2.26                     | 0.71              |
| 47:2m:1623:A:O4'  | 60:2z:133:GLY:HA3  | 1.90                     | 0.71              |
| 47:2m:1804:U:O4   | 81:2m:1901:84D:N4  | 2.23                     | 0.71              |
| 70:3H:201:LYS:O   | 70:3H:205:GLU:HG3  | 1.90                     | 0.71              |
| 1:1A:188:G:N2     | 1:1A:190:G:O6      | 2.23                     | 0.71              |
| 1:1A:300:A:H2'    | 1:1A:301:G:H8      | 1.56                     | 0.71              |
| 1:1A:1326:A:OP2   | 1:1A:4445:U:O2'    | 2.08                     | 0.71              |
| 1:1A:2469:C:H5'   | 1:1A:2470:C:OP2    | 1.89                     | 0.71              |
| 1:1A:4749:C:C3'   | 1:1A:4750:G:H5''   | 2.20                     | 0.71              |
| 1:1A:4993:G:N1    | 1:1A:5058:A:H2     | 1.85                     | 0.71              |
| 13:2E:118:LYS:HD2 | 13:2E:119:TYR:N    | 2.06                     | 0.71              |
| 17:2I:47:PHE:CE1  | 17:2I:140:ARG:HG2  | 2.26                     | 0.71              |
| 22:2N:85:LEU:HD11 | 22:2N:87:LYS:HD3   | 1.71                     | 0.71              |
| 39:2e:51:GLU:O    | 39:2e:54:GLU:HG2   | 1.91                     | 0.71              |
| 47:2m:1283:C:H5   | 72:3J:104:VAL:HG11 | 1.55                     | 0.71              |
| 48:2n:21:ALA:HB2  | 59:2y:91:LEU:HD11  | 1.72                     | 0.71              |
| 51:2q:139:LEU:CD2 | 51:2q:147:ILE:HB   | 2.20                     | 0.71              |
| 56:2v:30:LYS:HG2  | 56:2v:31:GLU:H     | 1.56                     | 0.71              |
| 68:3F:10:THR:HB   | 68:3F:306:LEU:HD11 | 1.72                     | 0.71              |
| 68:3F:106:LYS:HE3 | 68:3F:125:ARG:HB3  | 1.73                     | 0.71              |
| 76:3N:35:VAL:HG13 | 76:3N:40:ILE:HD11  | 1.72                     | 0.71              |
| 78:3P:33:MET:HE1  | 78:3P:73:LEU:HD21  | 1.71                     | 0.71              |
| 1:1A:1942:A:H2'   | 1:1A:1943:A:C8     | 2.26                     | 0.70              |
| 1:1A:3822:U:H2'   | 1:1A:3823:G:C8     | 2.26                     | 0.70              |
| 5:1E:17:LEU:HD21  | 5:1E:264:PHE:CD2   | 2.25                     | 0.70              |
| 47:2m:613:G:N1    | 47:2m:629:A:OP1    | 2.24                     | 0.70              |
| 47:2m:1448:A:O2'  | 47:2m:1449:G:O5'   | 2.08                     | 0.70              |
| 47:2m:1592:C:O2'  | 58:2x:44:PRO:HB3   | 1.91                     | 0.70              |
| 47:2m:1597:C:H4'  | 47:2m:1603:G:C6    | 2.26                     | 0.70              |
| 48:2n:63:ARG:HG2  | 48:2n:185:MET:HE1  | 1.71                     | 0.70              |
| 56:2v:33:LEU:HD12 | 56:2v:34:PRO:CD    | 2.19                     | 0.70              |
| 59:2y:25:GLY:O    | 59:2y:31:ASN:ND2   | 2.22                     | 0.70              |
| 70:3H:139:SER:O   | 70:3H:142:ARG:HG2  | 1.91                     | 0.70              |
| 1:1A:1770:A:H2'   | 1:1A:1771:U:C6     | 2.25                     | 0.70              |
| 1:1A:2547:G:O2'   | 1:1A:2548:C:H5'    | 1.90                     | 0.70              |
| 24:2P:99:GLU:HG3  | 25:2Q:21:TYR:OH    | 1.90                     | 0.70              |
| 47:2m:439:A:O2'   | 47:2m:440:G:H5'    | 1.90                     | 0.70              |
| 47:2m:1199:A:H2'  | 47:2m:1200:A:C8    | 2.26                     | 0.70              |
| 52:2r:16:ASP:N    | 52:2r:26:ASP:OD2   | 2.24                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 60:2z:142:ARG:O   | 60:2z:142:ARG:HD2  | 1.91                     | 0.70              |
| 1:1A:184:U:H5     | 1:1A:254:G:H2'     | 1.54                     | 0.70              |
| 1:1A:1563:A:N6    | 47:2m:1028:A:N1    | 2.39                     | 0.70              |
| 1:1A:2668:G:C2'   | 1:1A:2669:C:H5'    | 2.21                     | 0.70              |
| 8:1H:150:LEU:HD13 | 8:1H:194:VAL:HG11  | 1.71                     | 0.70              |
| 18:2J:4:TYR:OH    | 18:2J:18:ARG:HG3   | 1.91                     | 0.70              |
| 47:2m:698:G:O2'   | 47:2m:731:G:O6     | 2.08                     | 0.70              |
| 47:2m:875:A:H5'   | 53:2s:111:LYS:HE3  | 1.73                     | 0.70              |
| 47:2m:1257:G:H4'  | 47:2m:1258:A:C5'   | 2.21                     | 0.70              |
| 47:2m:1630:A:H5'' | 60:2z:37:GLY:N     | 2.06                     | 0.70              |
| 47:2m:1753:C:H5'' | 47:2m:1754:G:OP1   | 1.91                     | 0.70              |
| 48:2n:34:MET:HE1  | 48:2n:162:PRO:CB   | 2.21                     | 0.70              |
| 68:3F:8:ARG:HH21  | 68:3F:47:ARG:HA    | 1.56                     | 0.70              |
| 46:2l:131:ALA:HB3 | 46:2l:133:LYS:HE3  | 1.72                     | 0.70              |
| 47:2m:1648:G:H5'' | 58:2x:125:ARG:HB3  | 1.74                     | 0.70              |
| 47:2m:1863:A:H1'  | 65:3C:79:ILE:HD13  | 1.72                     | 0.70              |
| 49:2o:62:LEU:HD13 | 49:2o:96:CYS:SG    | 2.31                     | 0.70              |
| 57:2w:33:LEU:HD12 | 57:2w:36:LEU:HD12  | 1.73                     | 0.70              |
| 72:3J:30:GLY:O    | 72:3J:31:LEU:HD23  | 1.89                     | 0.70              |
| 1:1A:2574:G:N1    | 1:1A:2762:G:O6     | 2.19                     | 0.70              |
| 1:1A:4233:A:H4'   | 43:2i:98:LYS:CE    | 2.19                     | 0.70              |
| 1:1A:4317:A:H2'   | 1:1A:4318:C:C6     | 2.27                     | 0.70              |
| 6:1F:334:THR:HG21 | 9:2A:51:TYR:OH     | 1.91                     | 0.70              |
| 8:1H:96:VAL:HG12  | 8:1H:104:THR:HA    | 1.72                     | 0.70              |
| 8:1H:147:GLY:CA   | 8:1H:203:ILE:HG12  | 2.22                     | 0.70              |
| 12:2D:91:LEU:HD12 | 12:2D:135:ILE:HG23 | 1.73                     | 0.70              |
| 27:2S:2:LYS:HD3   | 27:2S:7:VAL:HG23   | 1.73                     | 0.70              |
| 47:2m:16:G:H2'    | 47:2m:17:C:C6      | 2.26                     | 0.70              |
| 47:2m:573:U:N3    | 47:2m:576:A:OP2    | 2.18                     | 0.70              |
| 47:2m:1264:C:C4'  | 47:2m:1265:A:H5'   | 2.21                     | 0.70              |
| 47:2m:1521:C:O2'  | 47:2m:1522:A:OP2   | 2.08                     | 0.70              |
| 47:2m:1538:C:H2'  | 47:2m:1539:U:C6    | 2.25                     | 0.70              |
| 47:2m:1755:C:H2'  | 47:2m:1756:C:C6    | 2.27                     | 0.70              |
| 55:2u:95:ARG:O    | 55:2u:95:ARG:NH1   | 2.22                     | 0.70              |
| 59:2y:17:ILE:HD12 | 59:2y:58:MET:HE1   | 1.72                     | 0.70              |
| 76:3N:5:VAL:O     | 76:3N:43:LYS:NZ    | 2.25                     | 0.70              |
| 77:3O:69:THR:O    | 77:3O:73:VAL:HG12  | 1.90                     | 0.70              |
| 1:1A:180:C:H2'    | 1:1A:181:C:C1'     | 2.21                     | 0.70              |
| 7:1G:264:LYS:HD3  | 7:1G:266:TRP:CZ2   | 2.26                     | 0.70              |
| 23:2O:95:ASN:O    | 23:2O:95:ASN:ND2   | 2.20                     | 0.70              |
| 25:2Q:80:ARG:NH2  | 70:3H:129:VAL:HG23 | 2.05                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:2a:103:VAL:O   | 35:2a:106:VAL:HG12 | 1.92                     | 0.70              |
| 47:2m:64:A:H2     | 47:2m:83:A:H62     | 1.38                     | 0.70              |
| 47:2m:1281:G:O2'  | 47:2m:1282:A:OP2   | 2.09                     | 0.70              |
| 47:2m:1822:A:H2'  | 47:2m:1823:A:C8    | 2.26                     | 0.70              |
| 52:2r:119:SER:O   | 52:2r:193:LYS:HG3  | 1.91                     | 0.70              |
| 60:2z:78:LYS:HE2  | 61:20:32:GLU:OE2   | 1.92                     | 0.70              |
| 63:3A:35:ASN:OD1  | 63:3A:52:THR:OG1   | 2.09                     | 0.70              |
| 70:3H:69:THR:O    | 70:3H:99:GLY:HA3   | 1.90                     | 0.70              |
| 1:1A:3726:A:H2'   | 1:1A:3727:A:C8     | 2.27                     | 0.70              |
| 1:1A:4095:G:H2'   | 1:1A:4096:C:C6     | 2.27                     | 0.70              |
| 1:1A:4731:G:O2'   | 1:1A:4732:G:OP2    | 2.06                     | 0.70              |
| 6:1F:8:ILE:HD11   | 6:1F:153:VAL:CG2   | 2.21                     | 0.70              |
| 8:1H:208:ILE:HG23 | 8:1H:212:LEU:HD12  | 1.74                     | 0.70              |
| 14:2F:197:LYS:O   | 14:2F:201:GLU:HG2  | 1.91                     | 0.70              |
| 47:2m:1648:G:C8   | 58:2x:17:LYS:HE3   | 2.26                     | 0.70              |
| 53:2s:84:GLU:OE2  | 53:2s:91:HIS:HA    | 1.91                     | 0.70              |
| 57:2w:93:MET:CE   | 57:2w:104:GLN:HB3  | 2.22                     | 0.70              |
| 62:21:24:LEU:HD13 | 62:21:32:LEU:CD1   | 2.21                     | 0.70              |
| 1:1A:2465:C:H1'   | 1:1A:3672:G:N2     | 2.03                     | 0.70              |
| 1:1A:4749:C:H2'   | 1:1A:4750:G:H5''   | 1.74                     | 0.70              |
| 46:2l:54:ARG:HE   | 46:2l:152:LYS:HE3  | 1.55                     | 0.70              |
| 48:2n:41:ARG:HD2  | 48:2n:47:TYR:CZ    | 2.26                     | 0.70              |
| 48:2n:153:PRO:O   | 48:2n:154:LEU:HD23 | 1.92                     | 0.70              |
| 52:2r:50:PRO:HB3  | 52:2r:69:VAL:CG1   | 2.22                     | 0.70              |
| 57:2w:56:LEU:HG   | 57:2w:60:LEU:HD21  | 1.74                     | 0.70              |
| 68:3F:168:CYS:HB2 | 68:3F:195:LEU:HD13 | 1.74                     | 0.70              |
| 73:3K:100:LYS:HA  | 73:3K:103:GLU:CD   | 2.17                     | 0.70              |
| 1:1A:1419:G:O2'   | 29:2U:116:LYS:NZ   | 2.23                     | 0.70              |
| 1:1A:3945:A:C2'   | 1:1A:3946:G:H5''   | 2.21                     | 0.70              |
| 12:2D:76:MET:HE2  | 12:2D:148:VAL:HA   | 1.71                     | 0.70              |
| 26:2R:64:SER:OG   | 36:2b:82:ASP:OD2   | 2.03                     | 0.70              |
| 32:2X:22:THR:HG22 | 32:2X:122:VAL:HB   | 1.73                     | 0.70              |
| 37:2c:73:ILE:O    | 37:2c:77:VAL:HG22  | 1.92                     | 0.70              |
| 47:2m:1024:A:O2'  | 47:2m:1025:U:H5'   | 1.91                     | 0.70              |
| 47:2m:1396:A:O2'  | 47:2m:1398:G:N7    | 2.24                     | 0.70              |
| 47:2m:1667:U:H2'  | 47:2m:1668:U:C6    | 2.26                     | 0.70              |
| 52:2r:91:ARG:HA   | 52:2r:94:LYS:HE3   | 1.74                     | 0.70              |
| 59:2y:87:GLU:OE1  | 59:2y:87:GLU:N     | 2.24                     | 0.70              |
| 1:1A:74:G:H5'     | 14:2F:59:VAL:CG1   | 2.21                     | 0.70              |
| 1:1A:3941:G:C2'   | 1:1A:3942:A:H5'    | 2.22                     | 0.70              |
| 43:2i:56:PHE:CE1  | 43:2i:58:LYS:HB2   | 2.27                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:493:A:C1'    | 47:2m:574:A:H5'    | 2.20                     | 0.70              |
| 47:2m:1434:C:H2'   | 47:2m:1435:C:C5    | 2.26                     | 0.70              |
| 76:3N:27:VAL:HB    | 76:3N:69:THR:CG2   | 2.22                     | 0.70              |
| 1:1A:982:U:OP1     | 8:1H:73:TYR:OH     | 2.09                     | 0.69              |
| 1:1A:1100:U:O3'    | 1:1A:1167:C:N4     | 2.25                     | 0.69              |
| 1:1A:4635:A:O2'    | 1:1A:4637:G:OP1    | 2.10                     | 0.69              |
| 8:1H:241:GLU:OE1   | 8:1H:241:GLU:HA    | 1.92                     | 0.69              |
| 28:2T:76:ASN:OD1   | 28:2T:77:TYR:N     | 2.25                     | 0.69              |
| 36:2b:4:ILE:CD1    | 36:2b:9:LEU:HD11   | 2.21                     | 0.69              |
| 39:2e:5:ILE:HD11   | 39:2e:43:TYR:HB3   | 1.72                     | 0.69              |
| 47:2m:562:U:H1'    | 71:3I:132:GLN:OE1  | 1.92                     | 0.69              |
| 47:2m:1433:C:H3'   | 47:2m:1434:C:C6    | 2.27                     | 0.69              |
| 47:2m:1664:A:O2'   | 47:2m:1665:G:OP1   | 2.09                     | 0.69              |
| 57:2w:75:VAL:HG13  | 57:2w:93:MET:SD    | 2.31                     | 0.69              |
| 57:2w:81:ARG:NH2   | 57:2w:117:GLY:O    | 2.25                     | 0.69              |
| 57:2w:90:VAL:HA    | 57:2w:107:ILE:CG2  | 2.22                     | 0.69              |
| 59:2y:24:LEU:HD11  | 59:2y:58:MET:HG2   | 1.72                     | 0.69              |
| 68:3F:154:VAL:O    | 68:3F:155:ARG:NH1  | 2.25                     | 0.69              |
| 70:3H:88:ARG:HG2   | 70:3H:91:GLU:HB2   | 1.74                     | 0.69              |
| 1:1A:956:A:H1'     | 1:1A:2076:G:H5''   | 1.75                     | 0.69              |
| 1:1A:1186:U:H2'    | 1:1A:1187:G:N3     | 2.07                     | 0.69              |
| 1:1A:3770:U:C2'    | 1:1A:3771:C:H5'    | 2.22                     | 0.69              |
| 1:1A:3938:G:H4'    | 1:1A:3939:G:O5'    | 1.91                     | 0.69              |
| 3:1C:82:A:OP2      | 3:1C:82:A:H4'      | 1.92                     | 0.69              |
| 4:1D:36:GLU:OE2    | 4:1D:163:ARG:NH1   | 2.23                     | 0.69              |
| 4:1D:186:TYR:HB2   | 4:1D:196:TRP:CZ3   | 2.27                     | 0.69              |
| 46:2l:147:LYS:HE2  | 46:2l:151:VAL:HG22 | 1.74                     | 0.69              |
| 47:2m:1301:A:H2'   | 47:2m:1303:C:H6    | 1.56                     | 0.69              |
| 52:2r:39:ILE:HG23  | 52:2r:41:VAL:HG12  | 1.73                     | 0.69              |
| 54:2t:137:LEU:HD23 | 54:2t:138:ASN:H    | 1.56                     | 0.69              |
| 55:2u:91:PRO:HD2   | 55:2u:94:LEU:HD23  | 1.74                     | 0.69              |
| 59:2y:57:LEU:O     | 59:2y:61:ILE:HG12  | 1.92                     | 0.69              |
| 1:1A:449:C:H4'     | 1:1A:450:G:OP2     | 1.92                     | 0.69              |
| 1:1A:1586:G:O2'    | 1:1A:1587:G:H5'    | 1.92                     | 0.69              |
| 47:2m:78:C:OP1     | 70:3H:173:ALA:HB3  | 1.93                     | 0.69              |
| 47:2m:1016:U:O2    | 73:3K:61:ALA:HB1   | 1.92                     | 0.69              |
| 48:2n:60:LEU:HD13  | 63:3A:79:VAL:HG22  | 1.73                     | 0.69              |
| 49:2o:224:GLU:HG2  | 49:2o:227:LYS:H    | 1.55                     | 0.69              |
| 50:2p:18:LYS:O     | 50:2p:21:LEU:HG    | 1.92                     | 0.69              |
| 50:2p:213:PRO:HD3  | 59:2y:19:LYS:HE3   | 1.74                     | 0.69              |
| 59:2y:92:ASP:N     | 59:2y:92:ASP:OD1   | 2.24                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:3A:55:ILE:HG21  | 63:3A:65:SER:OG    | 1.92                     | 0.69              |
| 68:3F:242:SER:HB3  | 68:3F:245:ARG:O    | 1.92                     | 0.69              |
| 1:1A:2318:G:N2     | 1:1A:2321:G:OP2    | 2.18                     | 0.69              |
| 1:1A:2823:G:O2'    | 1:1A:2824:C:H5'    | 1.93                     | 0.69              |
| 5:1E:394:LYS:O     | 5:1E:397:ILE:HG13  | 1.93                     | 0.69              |
| 7:1G:150:LEU:HD12  | 13:2E:146:ARG:HG3  | 1.73                     | 0.69              |
| 24:2P:106:VAL:HG12 | 24:2P:112:MET:HA   | 1.74                     | 0.69              |
| 47:2m:1277:C:OP1   | 55:2u:51:SER:OG    | 2.07                     | 0.69              |
| 54:2t:117:TYR:CD1  | 54:2t:156:ALA:HB2  | 2.28                     | 0.69              |
| 58:2x:32:ILE:HG23  | 58:2x:39:LEU:CD2   | 2.21                     | 0.69              |
| 61:20:116:ASP:OD1  | 61:20:117:GLN:N    | 2.25                     | 0.69              |
| 68:3F:225:LYS:HG3  | 68:3F:226:HIS:H    | 1.57                     | 0.69              |
| 72:3J:49:LEU:HA    | 72:3J:74:ILE:CG2   | 2.21                     | 0.69              |
| 77:3O:56:ASP:O     | 77:3O:60:LYS:HG2   | 1.91                     | 0.69              |
| 1:1A:2583:C:OP2    | 35:2a:76:ARG:NH1   | 2.26                     | 0.69              |
| 1:1A:2692:U:O2     | 39:2e:2:PRO:HB2    | 1.93                     | 0.69              |
| 1:1A:4120:U:H3'    | 1:1A:4121:G:H5''   | 1.75                     | 0.69              |
| 1:1A:4661:G:OP1    | 81:1A:5104:84D:N4  | 2.25                     | 0.69              |
| 2:1B:23:A:HO2'     | 2:1B:24:C:H6       | 1.37                     | 0.69              |
| 3:1C:87:G:H1'      | 3:1C:88:A:OP2      | 1.92                     | 0.69              |
| 3:1C:127:U:H2'     | 3:1C:128:C:H6      | 1.57                     | 0.69              |
| 16:2H:146:PRO:HB2  | 36:2b:104:THR:HG23 | 1.73                     | 0.69              |
| 20:2L:178:GLN:HA   | 20:2L:181:LYS:CE   | 2.20                     | 0.69              |
| 47:2m:156:G:H2'    | 47:2m:157:U:C6     | 2.28                     | 0.69              |
| 47:2m:465:A:H5'    | 47:2m:466:G:C5     | 2.27                     | 0.69              |
| 47:2m:1338:G:H4'   | 62:21:74:SER:H     | 1.56                     | 0.69              |
| 75:3M:57:ARG:H     | 75:3M:57:ARG:HD2   | 1.57                     | 0.69              |
| 1:1A:702:U:H3'     | 1:1A:703:G:H5''    | 1.74                     | 0.69              |
| 1:1A:4740:G:C2     | 1:1A:4741:C:H1'    | 2.27                     | 0.69              |
| 6:1F:292:ILE:O     | 6:1F:298:ILE:HD12  | 1.92                     | 0.69              |
| 47:2m:1146:C:OP1   | 65:3C:89:ARG:NH1   | 2.25                     | 0.69              |
| 47:2m:1446:A:O2'   | 47:2m:1447:G:H5''  | 1.92                     | 0.69              |
| 54:2t:123:ARG:HD2  | 54:2t:129:LEU:HD21 | 1.74                     | 0.69              |
| 59:2y:10:LYS:HG2   | 59:2y:53:TYR:CE2   | 2.28                     | 0.69              |
| 61:20:44:GLU:OE1   | 61:20:44:GLU:HA    | 1.91                     | 0.69              |
| 73:3K:102:LEU:HD21 | 73:3K:111:ALA:HB1  | 1.75                     | 0.69              |
| 1:1A:418:A:H61     | 3:1C:16:G:H1'      | 1.57                     | 0.69              |
| 1:1A:2765:A:C2'    | 1:1A:2766:A:H5'    | 2.22                     | 0.69              |
| 1:1A:4426:C:C2'    | 1:1A:4427:G:H5'    | 2.23                     | 0.69              |
| 1:1A:4694:G:H4'    | 11:2C:71:ARG:NH1   | 2.07                     | 0.69              |
| 4:1D:103:PRO:HG2   | 4:1D:106:THR:HG23  | 1.74                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:155:GLY:O     | 8:1H:158:ARG:HG3   | 1.92                     | 0.69              |
| 46:2l:74:CYS:O     | 46:2l:78:LYS:HG2   | 1.92                     | 0.69              |
| 46:2l:91:LYS:HG2   | 46:2l:124:LEU:HG   | 1.74                     | 0.69              |
| 47:2m:1402:A:O2'   | 62:21:54:VAL:HG21  | 1.92                     | 0.69              |
| 47:2m:1630:A:H5''  | 60:2z:37:GLY:H     | 1.57                     | 0.69              |
| 47:2m:1745:A:H2'   | 70:3H:65:GLN:OE1   | 1.93                     | 0.69              |
| 47:2m:1814:G:H5'   | 47:2m:1815:A:OP1   | 1.92                     | 0.69              |
| 48:2n:118:GLU:O    | 69:3G:65:LYS:NZ    | 2.21                     | 0.69              |
| 50:2p:55:THR:HA    | 50:2p:58:VAL:CG1   | 2.22                     | 0.69              |
| 52:2r:102:LEU:HD11 | 77:3O:108:ILE:CG2  | 2.23                     | 0.69              |
| 52:2r:164:ARG:O    | 77:3O:41:ARG:NH2   | 2.25                     | 0.69              |
| 70:3H:64:LYS:HE2   | 70:3H:82:SER:HB3   | 1.74                     | 0.69              |
| 73:3K:29:THR:N     | 73:3K:32:ASP:OD2   | 2.25                     | 0.69              |
| 1:1A:484:U:H4'     | 1:1A:485:C:C5'     | 2.23                     | 0.69              |
| 1:1A:1333:A:H2'    | 1:1A:1334:A:C8     | 2.27                     | 0.69              |
| 1:1A:1378:C:H4'    | 1:1A:1379:C:H5'    | 1.73                     | 0.69              |
| 1:1A:1754:U:H2'    | 1:1A:1755:C:C5     | 2.28                     | 0.69              |
| 1:1A:1791:U:H2'    | 1:1A:1792:U:H5'    | 1.73                     | 0.69              |
| 1:1A:2559:G:H2'    | 1:1A:2560:C:C6     | 2.27                     | 0.69              |
| 1:1A:4472:G:O2'    | 41:2g:100:TYR:O    | 2.11                     | 0.69              |
| 1:1A:5057:C:H2'    | 1:1A:5058:A:C8     | 2.27                     | 0.69              |
| 2:1B:55:A:O2'      | 13:2E:151:ILE:O    | 2.05                     | 0.69              |
| 14:2F:146:LEU:HD22 | 36:2b:122:LYS:HD3  | 1.75                     | 0.69              |
| 46:2l:70:ASP:O     | 46:2l:71:GLN:HG2   | 1.91                     | 0.69              |
| 46:2l:85:MET:HE3   | 46:2l:85:MET:O     | 1.93                     | 0.69              |
| 46:2l:118:LYS:O    | 46:2l:122:ARG:NH2  | 2.26                     | 0.69              |
| 47:2m:67:C:H42     | 70:3H:167:LYS:HB2  | 1.57                     | 0.69              |
| 47:2m:195:C:H2'    | 47:2m:196:C:C6     | 2.28                     | 0.69              |
| 47:2m:321:C:H2'    | 47:2m:322:C:C1'    | 2.23                     | 0.69              |
| 47:2m:517:C:H2'    | 47:2m:518:G:O4'    | 1.93                     | 0.69              |
| 47:2m:1228:A:H2'   | 47:2m:1229:G:C8    | 2.28                     | 0.69              |
| 47:2m:1378:A:OP2   | 48:2n:102:ARG:NH2  | 2.25                     | 0.69              |
| 47:2m:1713:C:O2'   | 47:2m:1714:U:H5'   | 1.93                     | 0.69              |
| 50:2p:158:ILE:HG23 | 50:2p:164:VAL:HG12 | 1.74                     | 0.69              |
| 52:2r:52:SER:HA    | 58:2x:50:LYS:HE3   | 1.75                     | 0.69              |
| 52:2r:128:ILE:HG12 | 66:3D:23:SER:OG    | 1.93                     | 0.69              |
| 53:2s:31:GLU:HB3   | 53:2s:37:LYS:HZ2   | 1.57                     | 0.69              |
| 53:2s:41:ARG:HG2   | 53:2s:42:GLU:HG2   | 1.73                     | 0.69              |
| 66:3D:14:VAL:HG23  | 66:3D:30:VAL:HB    | 1.72                     | 0.69              |
| 66:3D:31:ARG:HG3   | 66:3D:31:ARG:O     | 1.93                     | 0.69              |
| 68:3F:107:ASP:OD2  | 68:3F:125:ARG:NH1  | 2.26                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:3F:217:MET:HB3  | 68:3F:229:THR:HG23 | 1.74                     | 0.69              |
| 69:3G:183:LYS:HG3  | 75:3M:95:PRO:O     | 1.93                     | 0.69              |
| 76:3N:77:ASP:OD1   | 76:3N:78:SER:N     | 2.26                     | 0.69              |
| 1:1A:1468:C:OP1    | 29:2U:132:ARG:NH2  | 2.25                     | 0.69              |
| 1:1A:4412:C:H2'    | 1:1A:4413:C:O2     | 1.93                     | 0.69              |
| 46:2l:68:LEU:HD23  | 46:2l:82:ILE:CD1   | 2.23                     | 0.69              |
| 47:2m:604:A:H2'    | 47:2m:605:A:C8     | 2.28                     | 0.69              |
| 47:2m:983:A:C2     | 74:3L:139:SER:HB3  | 2.25                     | 0.69              |
| 47:2m:1419:C:O3'   | 61:20:129:ARG:HA   | 1.92                     | 0.69              |
| 64:3B:130:LEU:HA   | 64:3B:133:LEU:HD12 | 1.75                     | 0.69              |
| 68:3F:197:THR:HG21 | 68:3F:239:LEU:H    | 1.58                     | 0.69              |
| 1:1A:4132:C:O2'    | 1:1A:4133:C:H5'    | 1.93                     | 0.69              |
| 4:1D:196:TRP:HB3   | 4:1D:197:PRO:HD3   | 1.74                     | 0.69              |
| 46:2l:193:LEU:HG   | 46:2l:194:LEU:HD12 | 1.75                     | 0.69              |
| 47:2m:1290:G:H2'   | 47:2m:1291:A:O4'   | 1.92                     | 0.69              |
| 49:2o:62:LEU:O     | 49:2o:65:ARG:HG3   | 1.93                     | 0.69              |
| 52:2r:109:LEU:O    | 52:2r:113:VAL:HG13 | 1.93                     | 0.69              |
| 71:3l:84:ILE:HD11  | 71:3l:148:ILE:HG21 | 1.73                     | 0.69              |
| 1:1A:351:C:O2'     | 1:1A:352:G:H5'     | 1.93                     | 0.68              |
| 1:1A:513:U:N3      | 1:1A:516:C:OP2     | 2.26                     | 0.68              |
| 1:1A:2003:G:O2'    | 1:1A:2005:G:OP2    | 2.08                     | 0.68              |
| 4:1D:178:PRO:HG2   | 44:2j:26:VAL:HG23  | 1.75                     | 0.68              |
| 11:2C:10:VAL:HG21  | 11:2C:78:GLN:HG3   | 1.73                     | 0.68              |
| 14:2F:46:ILE:HD11  | 14:2F:51:ALA:HA    | 1.74                     | 0.68              |
| 25:2Q:96:GLN:HB2   | 25:2Q:100:VAL:HG11 | 1.74                     | 0.68              |
| 47:2m:92:A:H4'     | 47:2m:93:U:OP2     | 1.94                     | 0.68              |
| 47:2m:1513:C:H2'   | 47:2m:1514:G:H8    | 1.58                     | 0.68              |
| 50:2p:141:LYS:NZ   | 50:2p:179:GLN:HG2  | 2.08                     | 0.68              |
| 1:1A:1180:C:H4'    | 1:1A:1181:C:OP1    | 1.91                     | 0.68              |
| 1:1A:1827:C:O2'    | 1:1A:1828:C:H5'    | 1.94                     | 0.68              |
| 1:1A:2463:G:O2'    | 1:1A:2464:C:H5'    | 1.94                     | 0.68              |
| 1:1A:3736:A:H2'    | 1:1A:3737:A:H8     | 1.56                     | 0.68              |
| 1:1A:3953:G:H2'    | 1:1A:3954:A:C8     | 2.27                     | 0.68              |
| 2:1B:24:C:H2'      | 2:1B:25:G:O4'      | 1.93                     | 0.68              |
| 11:2C:41:ILE:HG22  | 11:2C:43:VAL:HG13  | 1.74                     | 0.68              |
| 31:2W:37:MET:HA    | 31:2W:37:MET:CE    | 2.19                     | 0.68              |
| 47:2m:878:G:O6     | 47:2m:908:A:C6     | 2.46                     | 0.68              |
| 47:2m:1126:G:OP1   | 48:2n:41:ARG:NH1   | 2.25                     | 0.68              |
| 47:2m:1377:U:H3'   | 48:2n:102:ARG:HH22 | 1.56                     | 0.68              |
| 47:2m:1671:G:O3'   | 58:2x:18:THR:OG1   | 2.11                     | 0.68              |
| 47:2m:1675:A:O2'   | 52:2r:74:ASN:HB3   | 1.93                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:2n:85:ARG:NE    | 48:2n:201:LEU:O    | 2.26                     | 0.68              |
| 48:2n:89:LYS:HB3   | 48:2n:202:TYR:CE1  | 2.28                     | 0.68              |
| 60:2z:30:ILE:CG1   | 60:2z:71:MET:HE1   | 2.23                     | 0.68              |
| 64:3B:32:LEU:HD11  | 64:3B:34:THR:HB    | 1.76                     | 0.68              |
| 65:3C:43:ASN:OD1   | 65:3C:45:VAL:HG23  | 1.94                     | 0.68              |
| 68:3F:8:ARG:NH2    | 68:3F:47:ARG:HA    | 2.08                     | 0.68              |
| 1:1A:2486:G:O6     | 1:1A:2493:G:O6     | 2.11                     | 0.68              |
| 1:1A:3597:G:H2'    | 1:1A:3598:C:C6     | 2.29                     | 0.68              |
| 1:1A:3944:G:H1     | 1:1A:4069:U:H3     | 0.77                     | 0.68              |
| 1:1A:4941:G:O2'    | 1:1A:4942:C:H5'    | 1.94                     | 0.68              |
| 12:2D:145:GLU:O    | 12:2D:148:VAL:HG22 | 1.94                     | 0.68              |
| 22:2N:43:LYS:O     | 22:2N:58:HIS:ND1   | 2.26                     | 0.68              |
| 47:2m:17:C:O2'     | 47:2m:1194:A:N1    | 2.26                     | 0.68              |
| 47:2m:659:G:H2'    | 47:2m:663:C:C6     | 2.28                     | 0.68              |
| 49:2o:26:SER:O     | 49:2o:51:ARG:NH2   | 2.26                     | 0.68              |
| 60:2z:73:ASN:ND2   | 60:2z:76:GLN:HB2   | 2.08                     | 0.68              |
| 72:3J:86:GLY:O     | 72:3J:89:VAL:HG12  | 1.93                     | 0.68              |
| 1:1A:266:C:OP1     | 1:1A:266:C:H3'     | 1.93                     | 0.68              |
| 1:1A:1095:A:H2'    | 1:1A:1096:C:C6     | 2.28                     | 0.68              |
| 1:1A:1455:G:O2'    | 1:1A:1456:C:H5'    | 1.93                     | 0.68              |
| 1:1A:1987:C:H2'    | 1:1A:1989:G:H22    | 1.58                     | 0.68              |
| 1:1A:2467:U:H4'    | 1:1A:2468:U:H5'    | 1.75                     | 0.68              |
| 1:1A:2764:A:H2'    | 1:1A:2765:A:C8     | 2.28                     | 0.68              |
| 1:1A:4107:G:O6     | 1:1A:4110:C:N4     | 2.27                     | 0.68              |
| 1:1A:4546:A:N7     | 4:1D:215:ASN:ND2   | 2.42                     | 0.68              |
| 1:1A:4869:U:C2'    | 1:1A:4870:G:H5'    | 2.23                     | 0.68              |
| 2:1B:110:G:H2'     | 2:1B:111:C:C6      | 2.29                     | 0.68              |
| 8:1H:281:ILE:CB    | 8:1H:286:LEU:HD21  | 2.23                     | 0.68              |
| 11:2C:173:ARG:HB3  | 41:2g:127:VAL:HG13 | 1.74                     | 0.68              |
| 36:2b:96:ASN:OD1   | 36:2b:99:GLU:HG3   | 1.92                     | 0.68              |
| 47:2m:95:G:H21     | 47:2m:474:G:H5'    | 1.59                     | 0.68              |
| 47:2m:1171:G:O2'   | 47:2m:1187:G:O6    | 2.11                     | 0.68              |
| 47:2m:1779:G:N2    | 47:2m:1780:G:O6    | 2.27                     | 0.68              |
| 49:2o:168:MET:HA   | 49:2o:197:ILE:HD12 | 1.74                     | 0.68              |
| 53:2s:101:LEU:CD2  | 53:2s:102:PRO:HD2  | 2.24                     | 0.68              |
| 69:3G:195:LEU:HD23 | 69:3G:224:THR:HG23 | 1.76                     | 0.68              |
| 76:3N:86:GLU:OE1   | 76:3N:87:PRO:HD2   | 1.94                     | 0.68              |
| 1:1A:23:C:H2'      | 1:1A:24:G:O4'      | 1.93                     | 0.68              |
| 1:1A:70:A:OP2      | 29:2U:64:LYS:HE3   | 1.92                     | 0.68              |
| 1:1A:326:C:O2'     | 1:1A:327:U:H5'     | 1.94                     | 0.68              |
| 1:1A:418:A:C2      | 3:1C:17:A:H1'      | 2.29                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:2M:17:LEU:HD11  | 22:2N:136:ARG:NH1  | 2.08                     | 0.68              |
| 35:2a:100:GLN:O    | 35:2a:103:VAL:HG22 | 1.93                     | 0.68              |
| 47:2m:125:C:H2'    | 70:3H:198:ARG:NH2  | 2.09                     | 0.68              |
| 47:2m:170:A:OP2    | 70:3H:140:ARG:NH1  | 2.25                     | 0.68              |
| 53:2s:9:VAL:HB     | 53:2s:44:ASN:OD1   | 1.92                     | 0.68              |
| 54:2t:141:ARG:CB   | 54:2t:145:ILE:HD11 | 2.24                     | 0.68              |
| 58:2x:19:ALA:HB2   | 58:2x:75:GLY:HA3   | 1.75                     | 0.68              |
| 61:20:23:LYS:HA    | 61:20:54:TYR:CE2   | 2.27                     | 0.68              |
| 63:3A:9:VAL:HG23   | 63:3A:9:VAL:O      | 1.92                     | 0.68              |
| 66:3D:15:THR:HG22  | 66:3D:31:ARG:O     | 1.93                     | 0.68              |
| 68:3F:248:LEU:HG   | 68:3F:259:TRP:O    | 1.93                     | 0.68              |
| 70:3H:176:ILE:HG22 | 70:3H:179:LEU:HB2  | 1.76                     | 0.68              |
| 77:3O:73:VAL:HG11  | 77:3O:88:LEU:CD1   | 2.23                     | 0.68              |
| 1:1A:265:C:HO2'    | 1:1A:266:C:P       | 2.16                     | 0.68              |
| 1:1A:2579:G:N2     | 1:1A:2582:A:OP2    | 2.26                     | 0.68              |
| 1:1A:2789:A:H1'    | 1:1A:2796:G:O4'    | 1.94                     | 0.68              |
| 6:1F:171:LEU:HD11  | 6:1F:177:TRP:CE3   | 2.27                     | 0.68              |
| 13:2E:29:SER:HB3   | 13:2E:67:LYS:O     | 1.94                     | 0.68              |
| 14:2F:49:ARG:O     | 14:2F:149:GLN:HG3  | 1.94                     | 0.68              |
| 29:2U:113:GLY:O    | 29:2U:136:LYS:NZ   | 2.21                     | 0.68              |
| 47:2m:1417:C:N3    | 61:20:128:GLN:NE2  | 2.39                     | 0.68              |
| 47:2m:1542:C:H4'   | 61:20:11:GLN:CB    | 2.24                     | 0.68              |
| 47:2m:1593:C:H1'   | 61:20:12:GLN:OE1   | 1.93                     | 0.68              |
| 52:2r:17:ILE:HD13  | 52:2r:46:ALA:HB3   | 1.75                     | 0.68              |
| 57:2w:111:MET:HB3  | 60:2z:117:ILE:HD11 | 1.74                     | 0.68              |
| 60:2z:109:GLU:O    | 60:2z:112:GLU:HG3  | 1.94                     | 0.68              |
| 66:3D:61:SER:O     | 66:3D:62:GLU:HG2   | 1.93                     | 0.68              |
| 1:1A:2743:A:H2'    | 1:1A:2744:A:C8     | 2.28                     | 0.68              |
| 1:1A:2859:G:N2     | 1:1A:3837:C:O2     | 2.26                     | 0.68              |
| 1:1A:3772:U:H2'    | 1:1A:3775:A:H2     | 1.59                     | 0.68              |
| 5:1E:17:LEU:HB3    | 5:1E:18:PRO:HD3    | 1.75                     | 0.68              |
| 7:1G:276:LYS:O     | 7:1G:280:VAL:HG12  | 1.94                     | 0.68              |
| 27:2S:47:MET:CE    | 27:2S:122:LYS:HD2  | 2.23                     | 0.68              |
| 46:2l:68:LEU:HD23  | 46:2l:82:ILE:HD12  | 1.74                     | 0.68              |
| 48:2n:20:ALA:HB1   | 59:2y:91:LEU:HA    | 1.76                     | 0.68              |
| 57:2w:67:ALA:HB2   | 57:2w:73:PRO:HB3   | 1.75                     | 0.68              |
| 59:2y:56:HIS:O     | 59:2y:59:LYS:HG2   | 1.92                     | 0.68              |
| 71:3I:125:HIS:O    | 71:3I:129:LEU:HG   | 1.94                     | 0.68              |
| 1:1A:1365:C:H2'    | 1:1A:1366:G:H5'    | 1.75                     | 0.68              |
| 1:1A:2611:A:H2'    | 1:1A:2612:G:H8     | 1.58                     | 0.68              |
| 1:1A:3960:A:H3'    | 1:1A:3961:G:C5'    | 2.23                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4717:A:O2'    | 1:1A:4718:G:H5'    | 1.93                     | 0.68              |
| 3:1C:144:U:H2'     | 3:1C:145:C:C6      | 2.29                     | 0.68              |
| 7:1G:60:ILE:HD11   | 7:1G:93:THR:HA     | 1.73                     | 0.68              |
| 10:2B:148:GLU:HA   | 10:2B:177:MET:HE2  | 1.76                     | 0.68              |
| 13:2E:120:ASP:HB2  | 13:2E:123:ILE:CG1  | 2.24                     | 0.68              |
| 17:2I:31:ARG:O     | 17:2I:33:VAL:HG23  | 1.94                     | 0.68              |
| 28:2T:103:ASP:OD1  | 28:2T:105:ALA:N    | 2.26                     | 0.68              |
| 52:2r:156:THR:O    | 52:2r:160:GLU:HG2  | 1.93                     | 0.68              |
| 54:2t:73:THR:O     | 54:2t:74:ARG:NH1   | 2.25                     | 0.68              |
| 54:2t:151:GLU:CA   | 54:2t:154:LYS:HE3  | 2.18                     | 0.68              |
| 70:3H:63:MET:HE3   | 70:3H:63:MET:CA    | 2.20                     | 0.68              |
| 1:1A:38:A:H5''     | 29:2U:35:ALA:HB2   | 1.75                     | 0.68              |
| 1:1A:993:G:H1      | 1:1A:1050:C:H2'    | 1.59                     | 0.68              |
| 1:1A:1726:U:H5'    | 9:2A:135:ILE:CD1   | 2.24                     | 0.68              |
| 1:1A:3759:A:H62    | 1:1A:3763:A:H2     | 1.42                     | 0.68              |
| 1:1A:4137:C:H2'    | 1:1A:4138:C:C6     | 2.28                     | 0.68              |
| 12:2D:54:SER:HB3   | 12:2D:135:ILE:CD1  | 2.19                     | 0.68              |
| 43:2i:11:PHE:O     | 43:2i:81:ARG:NH2   | 2.27                     | 0.68              |
| 47:2m:1604:G:H2'   | 47:2m:1605:G:H5'   | 1.76                     | 0.68              |
| 47:2m:1860:A:O5'   | 65:3C:8:ASN:HB3    | 1.94                     | 0.68              |
| 50:2p:23:GLU:OE1   | 50:2p:27:ARG:NH2   | 2.27                     | 0.68              |
| 52:2r:128:ILE:HG12 | 66:3D:23:SER:CB    | 2.23                     | 0.68              |
| 53:2s:31:GLU:HB2   | 53:2s:32:MET:HE1   | 1.75                     | 0.68              |
| 72:3J:64:LEU:CD1   | 80:3R:106:TYR:HB2  | 2.24                     | 0.68              |
| 74:3L:97:LEU:HD22  | 74:3L:98:ARG:H     | 1.59                     | 0.68              |
| 1:1A:2745:A:H2'    | 1:1A:2746:A:C8     | 2.28                     | 0.68              |
| 47:2m:417:C:O2'    | 47:2m:418:A:H5'    | 1.94                     | 0.68              |
| 47:2m:575:A:P      | 76:3N:89:HIS:HB2   | 2.34                     | 0.68              |
| 47:2m:1259:A:H62   | 47:2m:1518:C:H3'   | 1.59                     | 0.68              |
| 47:2m:1776:G:H2'   | 47:2m:1777:G:H8    | 1.59                     | 0.68              |
| 56:2v:3:ASP:OD1    | 56:2v:4:ILE:N      | 2.23                     | 0.68              |
| 59:2y:14:ARG:O     | 59:2y:18:GLU:HG2   | 1.94                     | 0.68              |
| 69:3G:104:ASP:HB3  | 69:3G:130:ILE:HD13 | 1.76                     | 0.68              |
| 69:3G:133:TYR:HA   | 69:3G:216:MET:O    | 1.94                     | 0.68              |
| 70:3H:199:THR:O    | 70:3H:203:LYS:HG2  | 1.94                     | 0.68              |
| 71:3I:45:ARG:O     | 71:3I:49:THR:HG23  | 1.94                     | 0.68              |
| 72:3J:16:THR:O     | 72:3J:20:GLU:HG2   | 1.94                     | 0.68              |
| 1:1A:266:C:H1'     | 1:1A:267:G:N7      | 2.09                     | 0.67              |
| 1:1A:1551:C:C2'    | 1:1A:1552:G:H5'    | 2.24                     | 0.67              |
| 1:1A:1719:A:H2'    | 1:1A:1720:C:C6     | 2.28                     | 0.67              |
| 1:1A:2539:C:H2'    | 1:1A:2540:C:C6     | 2.29                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2907:G:O2'   | 1:1A:3589:G:N2     | 2.25                     | 0.67              |
| 27:2S:4:ASN:HB3   | 27:2S:7:VAL:CG2    | 2.24                     | 0.67              |
| 32:2X:90:ARG:HD2  | 32:2X:102:LEU:HD23 | 1.75                     | 0.67              |
| 46:2l:48:ARG:CD   | 46:2l:49:PHE:H     | 2.06                     | 0.67              |
| 47:2m:98:C:OP2    | 47:2m:426:A:O2'    | 2.11                     | 0.67              |
| 53:2s:163:GLN:O   | 53:2s:167:GLU:HB3  | 1.94                     | 0.67              |
| 74:3L:46:ASP:OD1  | 74:3L:48:SER:N     | 2.25                     | 0.67              |
| 1:1A:184:U:H4'    | 1:1A:185:C:O5'     | 1.93                     | 0.67              |
| 1:1A:325:U:H2'    | 1:1A:326:C:C6      | 2.29                     | 0.67              |
| 1:1A:1463:C:O2'   | 1:1A:1464:C:H5'    | 1.94                     | 0.67              |
| 1:1A:1683:U:H2'   | 1:1A:1684:A:H8     | 1.58                     | 0.67              |
| 1:1A:2284:G:OP1   | 29:2U:7:LYS:NZ     | 2.26                     | 0.67              |
| 1:1A:4056:A:H2'   | 1:1A:4057:C:C5     | 2.29                     | 0.67              |
| 1:1A:4098:A:H62   | 1:1A:4099:G:H21    | 1.41                     | 0.67              |
| 1:1A:4099:G:H4'   | 1:1A:4111:U:C2     | 2.29                     | 0.67              |
| 1:1A:4865:C:H2'   | 1:1A:4866:C:C6     | 2.29                     | 0.67              |
| 25:2Q:67:ILE:O    | 25:2Q:70:LYS:HG2   | 1.94                     | 0.67              |
| 47:2m:604:A:H4'   | 47:2m:605:A:OP1    | 1.94                     | 0.67              |
| 47:2m:1453:C:O2'  | 47:2m:1454:A:O5'   | 2.04                     | 0.67              |
| 47:2m:1589:A:H4'  | 61:20:82:ARG:CG    | 2.24                     | 0.67              |
| 50:2p:45:ARG:NH1  | 50:2p:83:SER:HA    | 2.08                     | 0.67              |
| 53:2s:46:THR:HG21 | 53:2s:97:GLN:HG3   | 1.76                     | 0.67              |
| 60:2z:40:TYR:O    | 60:2z:44:VAL:HG13  | 1.94                     | 0.67              |
| 60:2z:63:GLU:O    | 60:2z:67:VAL:HG23  | 1.93                     | 0.67              |
| 61:20:38:LYS:HD3  | 61:20:41:LYS:CB    | 2.24                     | 0.67              |
| 62:21:61:LEU:O    | 62:21:81:GLN:HA    | 1.94                     | 0.67              |
| 70:3H:23:LYS:HD3  | 70:3H:41:LEU:HA    | 1.76                     | 0.67              |
| 71:3I:111:GLN:OE1 | 71:3I:130:ILE:HD12 | 1.94                     | 0.67              |
| 1:1A:3732:A:H2'   | 1:1A:3733:A:C8     | 2.29                     | 0.67              |
| 47:2m:528:A:H2'   | 47:2m:529:A:H8     | 1.58                     | 0.67              |
| 47:2m:897:U:H5''  | 47:2m:898:U:OP2    | 1.94                     | 0.67              |
| 47:2m:913:A:N6    | 53:2s:98:ARG:O     | 2.27                     | 0.67              |
| 50:2p:206:ASP:OD1 | 50:2p:206:ASP:N    | 2.25                     | 0.67              |
| 51:2q:246:LEU:HB2 | 51:2q:251:GLU:OE2  | 1.94                     | 0.67              |
| 52:2r:82:ASN:CB   | 52:2r:85:LYS:HD2   | 2.25                     | 0.67              |
| 77:3O:58:LEU:HA   | 77:3O:62:VAL:CG1   | 2.23                     | 0.67              |
| 1:1A:924:C:H2'    | 1:1A:925:C:C6      | 2.29                     | 0.67              |
| 1:1A:1418:C:O2'   | 1:1A:1419:G:H5'    | 1.94                     | 0.67              |
| 1:1A:1943:A:H2'   | 1:1A:1944:A:H5'    | 1.76                     | 0.67              |
| 1:1A:2253:A:H2    | 9:2A:26:ALA:HB3    | 1.58                     | 0.67              |
| 1:1A:3690:U:O2'   | 1:1A:3691:G:H5'    | 1.93                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4902:C:O2'   | 1:1A:4903:G:H5'    | 1.94                     | 0.67              |
| 3:1C:67:U:H2'     | 3:1C:68:G:H8       | 1.60                     | 0.67              |
| 46:2l:3:SER:CB    | 46:2l:213:PRO:HD3  | 2.24                     | 0.67              |
| 46:2l:48:ARG:NE   | 46:2l:48:ARG:HA    | 2.09                     | 0.67              |
| 47:2m:96:C:H2'    | 47:2m:97:U:C6      | 2.30                     | 0.67              |
| 47:2m:604:A:N3    | 47:2m:639:C:O2'    | 2.21                     | 0.67              |
| 47:2m:1421:A:C2'  | 61:20:2:PRO:HB2    | 2.23                     | 0.67              |
| 48:2n:143:PRO:HB3 | 63:3A:32:ILE:HD13  | 1.75                     | 0.67              |
| 51:2q:19:MET:HE2  | 51:2q:108:ARG:HD2  | 1.76                     | 0.67              |
| 53:2s:33:ASN:HB3  | 53:2s:36:LEU:HB3   | 1.76                     | 0.67              |
| 60:2z:89:ASP:HB3  | 60:2z:92:ASP:OD1   | 1.94                     | 0.67              |
| 61:20:125:PRO:HA  | 61:20:128:GLN:CD   | 2.20                     | 0.67              |
| 69:3G:77:SER:O    | 69:3G:80:GLU:N     | 2.24                     | 0.67              |
| 71:3I:124:HIS:NE2 | 79:3Q:35:ARG:HG3   | 2.09                     | 0.67              |
| 77:3O:97:ILE:CG2  | 77:3O:109:TYR:HB3  | 2.25                     | 0.67              |
| 1:1A:1:C:O2'      | 1:1A:2:G:OP2       | 2.11                     | 0.67              |
| 1:1A:1942:A:OP1   | 81:1A:5115:84D:O6  | 2.12                     | 0.67              |
| 1:1A:2001:G:N2    | 1:1A:2003:G:O6     | 2.27                     | 0.67              |
| 1:1A:2083:C:OP2   | 19:2K:14:ARG:NH2   | 2.24                     | 0.67              |
| 1:1A:4239:A:H2'   | 1:1A:4240:G:C8     | 2.28                     | 0.67              |
| 1:1A:4537:C:H2'   | 1:1A:4538:G:C8     | 2.29                     | 0.67              |
| 1:1A:4765:G:H1    | 1:1A:4869:U:H3     | 1.40                     | 0.67              |
| 14:2F:127:PHE:HA  | 14:2F:143:GLU:OE2  | 1.93                     | 0.67              |
| 46:2l:108:ASP:O   | 46:2l:133:LYS:HB2  | 1.94                     | 0.67              |
| 47:2m:327:G:H1'   | 47:2m:328:U:O4'    | 1.93                     | 0.67              |
| 47:2m:876:C:H3'   | 47:2m:878:G:O2'    | 1.95                     | 0.67              |
| 47:2m:1019:C:H2'  | 47:2m:1020:A:O4'   | 1.94                     | 0.67              |
| 47:2m:1712:A:H2'  | 47:2m:1713:C:C6    | 2.30                     | 0.67              |
| 50:2p:58:VAL:HG11 | 50:2p:88:ALA:HB1   | 1.76                     | 0.67              |
| 52:2r:35:LEU:HD21 | 52:2r:147:VAL:HG22 | 1.74                     | 0.67              |
| 53:2s:58:LYS:HG2  | 53:2s:90:LYS:HD2   | 1.76                     | 0.67              |
| 59:2y:56:HIS:HA   | 59:2y:59:LYS:CD    | 2.24                     | 0.67              |
| 1:1A:139:G:H3'    | 1:1A:140:G:H8      | 1.60                     | 0.67              |
| 1:1A:425:U:H4'    | 18:2J:6:LEU:HD21   | 1.77                     | 0.67              |
| 1:1A:1179:U:H3'   | 1:1A:1180:C:H5''   | 1.75                     | 0.67              |
| 1:1A:1683:U:H2'   | 1:1A:1684:A:C8     | 2.30                     | 0.67              |
| 1:1A:2553:A:H4'   | 1:1A:2554:U:OP1    | 1.95                     | 0.67              |
| 1:1A:3872:A:O2'   | 1:1A:3873:G:H5'    | 1.95                     | 0.67              |
| 1:1A:4637:G:H2'   | 1:1A:4638:U:C6     | 2.28                     | 0.67              |
| 6:1F:210:ILE:CG2  | 6:1F:232:VAL:HB    | 2.25                     | 0.67              |
| 6:1F:210:ILE:HG22 | 6:1F:232:VAL:HB    | 1.77                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:2B:116:ALA:O    | 10:2B:119:GLU:HG3  | 1.95                     | 0.67              |
| 36:2b:16:GLU:OE1   | 36:2b:16:GLU:HA    | 1.94                     | 0.67              |
| 47:2m:389:A:H2'    | 47:2m:390:C:C6     | 2.30                     | 0.67              |
| 47:2m:1015:U:O2'   | 73:3K:55:ARG:NH1   | 2.28                     | 0.67              |
| 49:2o:82:ARG:HD3   | 49:2o:103:MET:HE3  | 1.75                     | 0.67              |
| 52:2r:24:SER:O     | 52:2r:107:ASN:ND2  | 2.23                     | 0.67              |
| 53:2s:53:VAL:CG2   | 53:2s:175:GLY:HA3  | 2.25                     | 0.67              |
| 54:2t:53:LYS:HE3   | 54:2t:55:TYR:CE2   | 2.30                     | 0.67              |
| 57:2w:98:ASN:HB2   | 57:2w:122:THR:HG22 | 1.77                     | 0.67              |
| 59:2y:17:ILE:HD12  | 59:2y:58:MET:SD    | 2.34                     | 0.67              |
| 60:2z:74:PRO:O     | 60:2z:79:ILE:HB    | 1.94                     | 0.67              |
| 1:1A:1294:A:H1'    | 1:1A:1296:G:N1     | 2.08                     | 0.67              |
| 1:1A:1846:G:H2'    | 1:1A:1847:C:H6     | 1.60                     | 0.67              |
| 1:1A:2876:G:C8     | 44:2j:16:THR:HG22  | 2.30                     | 0.67              |
| 1:1A:4584:A:H2'    | 1:1A:4585:U:O4'    | 1.95                     | 0.67              |
| 1:1A:4744:A:H2'    | 1:1A:4745:G:C8     | 2.30                     | 0.67              |
| 1:1A:4744:A:H61    | 1:1A:4955:A:H61    | 1.40                     | 0.67              |
| 30:2V:91:ARG:HA    | 30:2V:91:ARG:HE    | 1.60                     | 0.67              |
| 47:2m:126:G:OP2    | 47:2m:126:G:N2     | 2.24                     | 0.67              |
| 47:2m:221:A:O2'    | 47:2m:222:U:H5'    | 1.95                     | 0.67              |
| 47:2m:613:G:OP1    | 79:3Q:11:LYS:NZ    | 2.21                     | 0.67              |
| 47:2m:1592:C:H1'   | 58:2x:44:PRO:HG3   | 1.76                     | 0.67              |
| 48:2n:78:SER:HB3   | 48:2n:87:VAL:HG21  | 1.76                     | 0.67              |
| 48:2n:85:ARG:HG3   | 48:2n:89:LYS:HE2   | 1.75                     | 0.67              |
| 48:2n:145:ILE:HG23 | 48:2n:159:ILE:HB   | 1.76                     | 0.67              |
| 68:3F:10:THR:HB    | 68:3F:306:LEU:CD1  | 2.25                     | 0.67              |
| 77:3O:50:PHE:HB2   | 77:3O:54:THR:OG1   | 1.95                     | 0.67              |
| 78:3P:8:LEU:O      | 78:3P:9:HIS:ND1    | 2.28                     | 0.67              |
| 1:1A:2520:C:H2'    | 1:1A:2521:G:H8     | 1.60                     | 0.67              |
| 1:1A:3971:G:O2'    | 1:1A:3973:G:O2'    | 2.00                     | 0.67              |
| 1:1A:4212:A:H4'    | 1:1A:4213:A:O5'    | 1.95                     | 0.67              |
| 46:2l:120:ILE:HB   | 46:2l:121:PRO:HD3  | 1.77                     | 0.67              |
| 47:2m:197:U:H3     | 47:2m:202:G:H1     | 1.41                     | 0.67              |
| 47:2m:1101:U:H2'   | 47:2m:1102:G:H8    | 1.58                     | 0.67              |
| 47:2m:1287:A:H2'   | 47:2m:1315:U:O2    | 1.94                     | 0.67              |
| 47:2m:1444:U:H2'   | 47:2m:1445:U:C6    | 2.30                     | 0.67              |
| 50:2p:126:ILE:HG21 | 50:2p:134:CYS:HB2  | 1.77                     | 0.67              |
| 50:2p:201:LYS:HE2  | 50:2p:201:LYS:H    | 1.60                     | 0.67              |
| 52:2r:163:PHE:CD2  | 52:2r:164:ARG:HG3  | 2.29                     | 0.67              |
| 54:2t:148:LYS:HG3  | 54:2t:149:TYR:HD1  | 1.59                     | 0.67              |
| 60:2z:105:ASN:O    | 60:2z:109:GLU:HG2  | 1.95                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:3F:124:SER:OG   | 68:3F:126:ASP:OD1  | 2.11                     | 0.67              |
| 70:3H:70:HIS:HA    | 70:3H:98:ARG:HH12  | 1.59                     | 0.67              |
| 76:3N:88:LYS:HB3   | 76:3N:97:TYR:CE2   | 2.30                     | 0.67              |
| 1:1A:2262:G:OP2    | 45:2k:98:ARG:NH2   | 2.23                     | 0.67              |
| 1:1A:4906:C:H2'    | 1:1A:4907:G:H8     | 1.59                     | 0.67              |
| 23:2O:40:GLU:OE2   | 23:2O:65:ARG:HD2   | 1.94                     | 0.67              |
| 47:2m:1116:C:H2'   | 47:2m:1117:C:C6    | 2.29                     | 0.67              |
| 47:2m:1142:G:N2    | 47:2m:1145:A:OP2   | 2.22                     | 0.67              |
| 47:2m:1518:C:P     | 47:2m:1519:U:H2'   | 2.35                     | 0.67              |
| 47:2m:1649:U:OP1   | 58:2x:128:GLU:N    | 2.28                     | 0.67              |
| 48:2n:140:VAL:HG23 | 48:2n:142:LEU:CD2  | 2.25                     | 0.67              |
| 50:2p:75:LYS:HD2   | 55:2u:21:MET:HA    | 1.76                     | 0.67              |
| 52:2r:24:SER:OG    | 52:2r:27:ASP:OD2   | 2.13                     | 0.67              |
| 58:2x:84:ILE:O     | 58:2x:88:ILE:HG23  | 1.95                     | 0.67              |
| 59:2y:5:ARG:HD3    | 59:2y:53:TYR:HB2   | 1.75                     | 0.67              |
| 73:3K:100:LYS:O    | 73:3K:103:GLU:HG2  | 1.95                     | 0.67              |
| 1:1A:1296:G:H2'    | 1:1A:1297:U:C6     | 2.30                     | 0.67              |
| 1:1A:2093:A:O2'    | 1:1A:2094:G:H5'    | 1.95                     | 0.67              |
| 1:1A:2571:C:O2'    | 1:1A:2572:C:H5'    | 1.95                     | 0.67              |
| 1:1A:2725:A:H1'    | 20:2L:93:VAL:HG11  | 1.77                     | 0.67              |
| 1:1A:3868:G:H22    | 1:1A:3900:G:H1'    | 1.58                     | 0.67              |
| 1:1A:4279:A:H5'    | 1:1A:4281:A:C1'    | 2.21                     | 0.67              |
| 3:1C:89:U:H2'      | 3:1C:90:C:C6       | 2.30                     | 0.67              |
| 47:2m:536:A:H3'    | 47:2m:537:C:O4'    | 1.94                     | 0.67              |
| 47:2m:693:A:N1     | 47:2m:738:C:H1'    | 2.11                     | 0.67              |
| 47:2m:1779:G:H2'   | 47:2m:1780:G:C8    | 2.30                     | 0.67              |
| 50:2p:76:ARG:CB    | 55:2u:22:VAL:HG11  | 2.25                     | 0.67              |
| 56:2v:25:LEU:HD22  | 56:2v:25:LEU:H     | 1.60                     | 0.67              |
| 56:2v:55:TYR:CD1   | 56:2v:115:PRO:HG2  | 2.30                     | 0.67              |
| 57:2w:111:MET:HB3  | 60:2z:117:ILE:CG1  | 2.25                     | 0.67              |
| 57:2w:127:LYS:NZ   | 57:2w:128:HIS:HB3  | 2.09                     | 0.67              |
| 60:2z:27:ALA:HA    | 60:2z:45:LEU:CD1   | 2.24                     | 0.67              |
| 66:3D:31:ARG:HB2   | 66:3D:43:ILE:CD1   | 2.25                     | 0.67              |
| 68:3F:59:LEU:HD22  | 68:3F:90:TRP:HE3   | 1.58                     | 0.67              |
| 69:3G:74:LYS:CE    | 69:3G:269:PHE:HB3  | 2.22                     | 0.67              |
| 69:3G:156:ILE:O    | 69:3G:160:LEU:HD23 | 1.94                     | 0.67              |
| 71:3I:59:GLU:O     | 71:3I:62:THR:HG22  | 1.93                     | 0.67              |
| 72:3J:17:ALA:HA    | 72:3J:20:GLU:OE2   | 1.95                     | 0.67              |
| 74:3L:19:PRO:HG2   | 74:3L:27:VAL:HG11  | 1.77                     | 0.67              |
| 1:1A:173:C:H5'     | 14:2F:129:ARG:HH21 | 1.60                     | 0.66              |
| 1:1A:2496:G:H2'    | 1:1A:2497:C:C6     | 2.29                     | 0.66              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:2719:C:O2'    | 1:1A:2720:C:H5'   | 1.95                     | 0.66              |
| 1:1A:3871:A:H2'    | 1:1A:3872:A:C8    | 2.28                     | 0.66              |
| 1:1A:4751:G:C2'    | 1:1A:4752:U:H5'   | 2.26                     | 0.66              |
| 1:1A:5004:C:H2'    | 1:1A:5005:G:O4'   | 1.95                     | 0.66              |
| 8:1H:50:LEU:HD21   | 8:1H:54:ILE:HG22  | 1.77                     | 0.66              |
| 14:2F:144:LEU:HD12 | 14:2F:145:LYS:N   | 2.09                     | 0.66              |
| 14:2F:211:LYS:HE2  | 46:2l:184:HIS:CB  | 2.23                     | 0.66              |
| 47:2m:331:C:N4     | 70:3H:186:GLN:OE1 | 2.27                     | 0.66              |
| 47:2m:496:C:H4'    | 51:2q:28:ALA:O    | 1.95                     | 0.66              |
| 47:2m:1269:G:H2'   | 47:2m:1270:G:C8   | 2.31                     | 0.66              |
| 47:2m:1588:A:H3'   | 47:2m:1588:A:OP2  | 1.95                     | 0.66              |
| 52:2r:134:VAL:O    | 52:2r:135:ARG:HD2 | 1.96                     | 0.66              |
| 57:2w:53:GLN:O     | 57:2w:57:LEU:HD12 | 1.95                     | 0.66              |
| 58:2x:32:ILE:HD12  | 58:2x:68:ILE:CG1  | 2.23                     | 0.66              |
| 60:2z:67:VAL:O     | 60:2z:70:ILE:HG13 | 1.96                     | 0.66              |
| 77:3O:69:THR:HG23  | 77:3O:72:VAL:CG1  | 2.25                     | 0.66              |
| 1:1A:247:G:H2'     | 1:1A:248:C:H6     | 1.60                     | 0.66              |
| 1:1A:1354:A:H4'    | 1:1A:1355:G:O5'   | 1.95                     | 0.66              |
| 1:1A:3861:A:H2'    | 1:1A:3862:A:H8    | 1.59                     | 0.66              |
| 1:1A:4740:G:O6     | 1:1A:4959:U:O2    | 2.13                     | 0.66              |
| 10:2B:112:GLN:O    | 10:2B:115:LEU:HG  | 1.94                     | 0.66              |
| 10:2B:187:LYS:CG   | 10:2B:198:THR:HB  | 2.24                     | 0.66              |
| 11:2C:14:GLU:H     | 11:2C:14:GLU:CD   | 2.03                     | 0.66              |
| 46:2l:60:ARG:HB2   | 46:2l:61:PRO:HD3  | 1.77                     | 0.66              |
| 47:2m:107:A:H2'    | 47:2m:108:G:C8    | 2.30                     | 0.66              |
| 47:2m:690:G:C2'    | 47:2m:691:G:H5''  | 2.25                     | 0.66              |
| 47:2m:1446:A:H1'   | 62:21:55:ARG:CD   | 2.22                     | 0.66              |
| 70:3H:3:LEU:HB3    | 70:3H:5:ILE:HD11  | 1.75                     | 0.66              |
| 73:3K:41:ALA:CB    | 73:3K:75:LEU:HD11 | 2.26                     | 0.66              |
| 1:1A:179:G:HO2'    | 1:1A:180:C:P      | 2.18                     | 0.66              |
| 1:1A:513:U:O2'     | 1:1A:646:G:O6     | 2.13                     | 0.66              |
| 1:1A:2096:G:H2'    | 1:1A:2096:G:N3    | 2.10                     | 0.66              |
| 1:1A:4936:G:O2'    | 1:1A:4937:C:H5'   | 1.96                     | 0.66              |
| 25:2Q:2:LYS:NZ     | 25:2Q:3:VAL:O     | 2.26                     | 0.66              |
| 47:2m:554:A:H5'    | 47:2m:555:A:OP1   | 1.95                     | 0.66              |
| 47:2m:560:A:O5'    | 71:3I:174:LYS:HE2 | 1.95                     | 0.66              |
| 47:2m:1489:A:H4'   | 47:2m:1490:G:OP2  | 1.95                     | 0.66              |
| 48:2n:42:LYS:HE2   | 48:2n:44:ASP:OD1  | 1.95                     | 0.66              |
| 50:2p:204:LEU:HB3  | 50:2p:206:ASP:OD1 | 1.96                     | 0.66              |
| 56:2v:60:CYS:SG    | 56:2v:114:SER:OG  | 2.50                     | 0.66              |
| 59:2y:17:ILE:HD11  | 59:2y:54:VAL:HG13 | 1.76                     | 0.66              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:3937:C:H2'    | 1:1A:3938:G:N2    | 2.10                     | 0.66              |
| 1:1A:4094:G:H2'    | 1:1A:4095:G:H8    | 1.60                     | 0.66              |
| 1:1A:4765:G:H22    | 1:1A:4869:U:H3    | 1.43                     | 0.66              |
| 25:2Q:45:ASN:HD22  | 25:2Q:46:PRO:HD2  | 1.60                     | 0.66              |
| 47:2m:14:C:H5'     | 69:3G:190:SER:OG  | 1.96                     | 0.66              |
| 47:2m:640:A:H2'    | 47:2m:641:A:C8    | 2.30                     | 0.66              |
| 47:2m:786:G:OP2    | 70:3H:231:ARG:HB2 | 1.96                     | 0.66              |
| 47:2m:1219:C:O4'   | 66:3D:24:GLN:HG2  | 1.94                     | 0.66              |
| 47:2m:1393:G:H2'   | 47:2m:1394:G:C8   | 2.31                     | 0.66              |
| 47:2m:1403:C:N4    | 47:2m:1436:C:H5'' | 2.10                     | 0.66              |
| 50:2p:168:VAL:HG22 | 50:2p:189:MET:HB3 | 1.76                     | 0.66              |
| 59:2y:21:TYR:HE1   | 59:2y:71:ILE:HD13 | 1.61                     | 0.66              |
| 68:3F:110:SER:HB2  | 68:3F:155:ARG:NH2 | 2.11                     | 0.66              |
| 70:3H:57:ASP:OD1   | 70:3H:58:LYS:N    | 2.28                     | 0.66              |
| 70:3H:222:GLU:O    | 70:3H:226:GLU:HG2 | 1.94                     | 0.66              |
| 73:3K:66:VAL:HG13  | 73:3K:67:THR:HG23 | 1.78                     | 0.66              |
| 1:1A:1220:G:O2'    | 1:1A:1221:G:O5'   | 2.06                     | 0.66              |
| 1:1A:3596:A:C2'    | 1:1A:3597:G:H5'   | 2.25                     | 0.66              |
| 1:1A:4924:C:H2'    | 1:1A:4925:U:N1    | 2.11                     | 0.66              |
| 47:2m:941:C:O2'    | 47:2m:942:G:H5'   | 1.96                     | 0.66              |
| 48:2n:23:THR:OG1   | 48:2n:170:SER:OG  | 2.08                     | 0.66              |
| 48:2n:31:ASP:HB3   | 48:2n:34:MET:HB2  | 1.78                     | 0.66              |
| 61:20:63:HIS:CE1   | 61:20:78:ILE:HD12 | 2.31                     | 0.66              |
| 66:3D:15:THR:O     | 66:3D:52:GLU:HG3  | 1.96                     | 0.66              |
| 73:3K:13:GLN:O     | 78:3P:20:LYS:NZ   | 2.22                     | 0.66              |
| 1:1A:385:A:H4'     | 1:1A:386:A:OP1    | 1.94                     | 0.66              |
| 1:1A:661:C:H2'     | 1:1A:662:C:H6     | 1.60                     | 0.66              |
| 1:1A:2306:G:H1'    | 1:1A:2332:A:N6    | 2.11                     | 0.66              |
| 1:1A:2762:G:O2'    | 1:1A:2763:U:H5''  | 1.95                     | 0.66              |
| 47:2m:1033:G:H1    | 47:2m:1080:A:HO2' | 0.67                     | 0.66              |
| 47:2m:1452:A:H5'   | 47:2m:1453:C:C4   | 2.30                     | 0.66              |
| 49:2o:129:THR:OG1  | 49:2o:133:TYR:HB2 | 1.95                     | 0.66              |
| 61:20:125:PRO:O    | 61:20:128:GLN:HG2 | 1.96                     | 0.66              |
| 64:3B:68:LYS:CB    | 64:3B:91:LEU:HD22 | 2.25                     | 0.66              |
| 1:1A:1339:U:H2'    | 1:1A:1340:C:C6    | 2.31                     | 0.66              |
| 1:1A:1727:U:OP1    | 9:2A:131:ASN:ND2  | 2.29                     | 0.66              |
| 1:1A:4749:C:C2'    | 1:1A:4750:G:H5''  | 2.25                     | 0.66              |
| 46:2l:25:ARG:HD3   | 46:2l:210:MET:SD  | 2.36                     | 0.66              |
| 46:2l:108:ASP:HA   | 46:2l:133:LYS:HD3 | 1.77                     | 0.66              |
| 47:2m:140:C:H42    | 47:2m:144:U:H1'   | 1.60                     | 0.66              |
| 47:2m:338:G:H3'    | 47:2m:339:A:H2'   | 1.76                     | 0.66              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 47:2m:1403:C:OP2   | 47:2m:1405:A:N6      | 2.24                     | 0.66              |
| 51:2q:138:HIS:NE2  | 51:2q:148:ARG:HG2    | 2.10                     | 0.66              |
| 52:2r:100:ILE:HD11 | 52:2r:174:ALA:HA     | 1.78                     | 0.66              |
| 55:2u:1:MET:HB3    | 55:2u:3:MET:HG2      | 1.76                     | 0.66              |
| 62:21:48:LEU:HD13  | 62:21:93:SER:HB2     | 1.78                     | 0.66              |
| 69:3G:61:MET:HG2   | 69:3G:61:MET:O       | 1.95                     | 0.66              |
| 69:3G:271:ASP:O    | 69:3G:274:VAL:HG22   | 1.96                     | 0.66              |
| 76:3N:111:LYS:CA   | 76:3N:114:MET:HE3    | 2.26                     | 0.66              |
| 1:1A:495:C:O4'     | 1:1A:659:G:N2        | 2.29                     | 0.66              |
| 1:1A:923:C:H2'     | 1:1A:925:C:H5        | 1.60                     | 0.66              |
| 1:1A:1753:G:H2'    | 1:1A:1754:U:C6       | 2.30                     | 0.66              |
| 1:1A:1967:A:N6     | 1:1A:2021:G:N7       | 2.43                     | 0.66              |
| 1:1A:3963:A:H3'    | 1:1A:3965:A:OP2      | 1.95                     | 0.66              |
| 1:1A:4413:C:O2'    | 1:1A:4414:A:H5'      | 1.95                     | 0.66              |
| 2:1B:119:U:C2      | 7:1G:261:VAL:HG11    | 2.30                     | 0.66              |
| 5:1E:56:ILE:HD13   | 5:1E:365:LEU:CD2     | 2.25                     | 0.66              |
| 11:2C:117:PHE:O    | 11:2C:120:GLU:HG2    | 1.96                     | 0.66              |
| 22:2N:85:LEU:CD1   | 22:2N:87:LYS:HD3     | 2.25                     | 0.66              |
| 24:2P:66:LYS:O     | 24:2P:73:ARG:NH1     | 2.28                     | 0.66              |
| 47:2m:57:U:H5''    | 47:2m:504:G:H1'      | 1.78                     | 0.66              |
| 47:2m:187:G:O6     | 47:2m:213:G:N1       | 2.29                     | 0.66              |
| 50:2p:20:GLU:O     | 50:2p:23:GLU:HG3     | 1.95                     | 0.66              |
| 54:2t:133:GLU:O    | 54:2t:136:ILE:HG22   | 1.96                     | 0.66              |
| 57:2w:75:VAL:HG21  | 57:2w:104:GLN:OE1    | 1.95                     | 0.66              |
| 69:3G:133:TYR:CD1  | 69:3G:216:MET:HA     | 2.30                     | 0.66              |
| 71:3I:137:VAL:HG12 | 71:3I:138[A]:ARG:HG3 | 1.76                     | 0.66              |
| 1:1A:1260:G:O2'    | 1:1A:1261:G:H5'      | 1.95                     | 0.66              |
| 1:1A:1721:G:H2'    | 1:1A:1722:C:C6       | 2.31                     | 0.66              |
| 1:1A:1943:A:C2'    | 1:1A:1944:A:H5'      | 2.25                     | 0.66              |
| 1:1A:2094:G:N3     | 1:1A:2094:G:H2'      | 2.11                     | 0.66              |
| 1:1A:4074:C:O2'    | 1:1A:4075:U:H5'      | 1.95                     | 0.66              |
| 10:2B:175:ARG:HD2  | 10:2B:175:ARG:C      | 2.21                     | 0.66              |
| 17:2I:27:VAL:CG1   | 17:2I:98:ALA:HB1     | 2.25                     | 0.66              |
| 25:2Q:74:ARG:NE    | 47:2m:1748:G:H5'     | 2.10                     | 0.66              |
| 43:2i:104:ILE:O    | 43:2i:105:GLN:HG3    | 1.95                     | 0.66              |
| 47:2m:363:A:N6     | 47:2m:400:C:O2'      | 2.28                     | 0.66              |
| 47:2m:374:G:H2'    | 47:2m:375:U:C6       | 2.31                     | 0.66              |
| 47:2m:566:U:H3'    | 47:2m:567:C:C6       | 2.31                     | 0.66              |
| 47:2m:1019:C:O2'   | 47:2m:1020:A:H5'     | 1.96                     | 0.66              |
| 47:2m:1745:A:N6    | 47:2m:1789:G:O2'     | 2.29                     | 0.66              |
| 70:3H:39:ASP:O     | 70:3H:46:LYS:NZ      | 2.29                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:3H:140:ARG:HA   | 70:3H:143:LYS:HE2  | 1.78                     | 0.66              |
| 72:3J:65:VAL:HG22  | 72:3J:69:LEU:HD12  | 1.77                     | 0.66              |
| 77:3O:63:PRO:O     | 77:3O:97:ILE:HD11  | 1.95                     | 0.66              |
| 1:1A:1625:G:H4'    | 1:1A:1626:G:O5'    | 1.96                     | 0.66              |
| 1:1A:2545:U:H5''   | 1:1A:2546:G:H4'    | 1.76                     | 0.66              |
| 1:1A:4232:U:H4'    | 1:1A:4233:A:O4'    | 1.96                     | 0.66              |
| 12:2D:200:VAL:HG13 | 12:2D:208:LYS:NZ   | 2.11                     | 0.66              |
| 25:2Q:77:LYS:O     | 25:2Q:77:LYS:HD3   | 1.96                     | 0.66              |
| 46:2I:92:LYS:HD3   | 46:2I:97:LYS:CG    | 2.23                     | 0.66              |
| 46:2I:147:LYS:HE2  | 46:2I:151:VAL:CG2  | 2.25                     | 0.66              |
| 47:2m:84:A:N3      | 47:2m:150:A:O2'    | 2.29                     | 0.66              |
| 47:2m:455:A:H2'    | 47:2m:456:C:C6     | 2.31                     | 0.66              |
| 47:2m:848:U:O2'    | 47:2m:849:A:H5'    | 1.95                     | 0.66              |
| 47:2m:1231:C:O2'   | 47:2m:1253:A:N6    | 2.29                     | 0.66              |
| 47:2m:1262:C:H5''  | 47:2m:1263:U:H5    | 1.60                     | 0.66              |
| 54:2t:125:LYS:HD3  | 54:2t:128:LYS:CE   | 2.26                     | 0.66              |
| 54:2t:161:LEU:HD13 | 54:2t:195:LEU:HD23 | 1.77                     | 0.66              |
| 68:3F:249:CYS:SG   | 68:3F:298:LEU:HD11 | 2.36                     | 0.66              |
| 72:3J:89:VAL:HG23  | 72:3J:109:VAL:HG11 | 1.77                     | 0.66              |
| 1:1A:1732:C:OP1    | 22:2N:43:LYS:NZ    | 2.29                     | 0.65              |
| 1:1A:1738:A:O2'    | 1:1A:1739:G:H5'    | 1.95                     | 0.65              |
| 1:1A:1872:G:O2'    | 1:1A:4219:A:N3     | 2.25                     | 0.65              |
| 1:1A:1958:A:H4'    | 1:1A:1962:A:H1'    | 1.78                     | 0.65              |
| 1:1A:3910:C:H2'    | 1:1A:3911:C:C6     | 2.31                     | 0.65              |
| 1:1A:4905:C:H2'    | 1:1A:4906:C:C6     | 2.30                     | 0.65              |
| 3:1C:102:G:OP2     | 3:1C:104:A:O2'     | 2.12                     | 0.65              |
| 47:2m:155:G:N2     | 70:3H:56:ASN:OD1   | 2.29                     | 0.65              |
| 47:2m:1566:G:O2'   | 47:2m:1568:C:N4    | 2.27                     | 0.65              |
| 51:2q:54:TYR:CD1   | 76:3N:13:MET:HE1   | 2.30                     | 0.65              |
| 53:2s:8:ILE:CD1    | 53:2s:9:VAL:HG13   | 2.26                     | 0.65              |
| 56:2v:18:GLN:HG2   | 56:2v:33:LEU:HD21  | 1.77                     | 0.65              |
| 58:2x:42:ILE:HG12  | 58:2x:51:LEU:HD13  | 1.78                     | 0.65              |
| 58:2x:135:PRO:HD3  | 58:2x:141:TYR:CD1  | 2.31                     | 0.65              |
| 60:2z:65:GLU:O     | 60:2z:69:THR:HG23  | 1.95                     | 0.65              |
| 66:3D:11:LEU:HD12  | 66:3D:55:VAL:CG2   | 2.26                     | 0.65              |
| 68:3F:301:GLY:HA2  | 68:3F:307:VAL:HG22 | 1.77                     | 0.65              |
| 78:3P:30:SER:HB3   | 78:3P:49:HIS:CD2   | 2.31                     | 0.65              |
| 1:1A:271:C:H2'     | 1:1A:272:U:H6      | 1.60                     | 0.65              |
| 1:1A:1590:C:H5''   | 1:1A:1591:U:O5'    | 1.97                     | 0.65              |
| 1:1A:2014:C:C5     | 1:1A:2015:U:H1'    | 2.31                     | 0.65              |
| 1:1A:2815:A:H2'    | 1:1A:2816:G:C8     | 2.32                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:3950:U:H5''   | 1:1A:3951:G:C8     | 2.31                     | 0.65              |
| 1:1A:4099:G:O2'    | 1:1A:4100:C:O5'    | 2.15                     | 0.65              |
| 1:1A:4701:A:H2'    | 1:1A:4702:G:H5'    | 1.76                     | 0.65              |
| 1:1A:4883:C:H4'    | 1:1A:4884:G:C5'    | 2.27                     | 0.65              |
| 7:1G:278:ASP:O     | 7:1G:282:GLN:HG2   | 1.97                     | 0.65              |
| 10:2B:211:ASP:OD1  | 10:2B:211:ASP:N    | 2.28                     | 0.65              |
| 13:2E:158:SER:HB3  | 13:2E:161:GLU:OE2  | 1.95                     | 0.65              |
| 31:2W:48:LEU:HD21  | 31:2W:60:ILE:HG21  | 1.77                     | 0.65              |
| 48:2n:10:MET:HE3   | 59:2y:109:LEU:HD21 | 1.77                     | 0.65              |
| 48:2n:66:VAL:HG22  | 48:2n:186:ARG:HD3  | 1.78                     | 0.65              |
| 48:2n:105:PRO:HA   | 48:2n:132:GLN:HE21 | 1.60                     | 0.65              |
| 51:2q:166:THR:HG22 | 51:2q:168:LYS:HG2  | 1.77                     | 0.65              |
| 51:2q:255:ARG:O    | 51:2q:259:LYS:HG2  | 1.96                     | 0.65              |
| 53:2s:43:LEU:HB2   | 53:2s:72:PHE:HE1   | 1.61                     | 0.65              |
| 56:2v:128:VAL:HG12 | 56:2v:142:VAL:HA   | 1.79                     | 0.65              |
| 71:3I:154:GLN:O    | 71:3I:157:ILE:HD12 | 1.95                     | 0.65              |
| 72:3J:64:LEU:HD11  | 80:3R:106:TYR:HB2  | 1.78                     | 0.65              |
| 1:1A:462:G:H2'     | 1:1A:463:A:C8      | 2.31                     | 0.65              |
| 1:1A:3903:A:H2'    | 1:1A:3904:G:O4'    | 1.96                     | 0.65              |
| 1:1A:3957:U:OP1    | 1:1A:3964:U:O2'    | 2.12                     | 0.65              |
| 1:1A:4670:C:O2'    | 1:1A:4672:A:OP2    | 2.08                     | 0.65              |
| 2:1B:49:A:OP1      | 7:1G:225:GLN:HB2   | 1.96                     | 0.65              |
| 15:2G:97:ALA:CB    | 17:2I:203:VAL:HG22 | 2.26                     | 0.65              |
| 22:2N:28:ALA:O     | 22:2N:32:ARG:HG2   | 1.96                     | 0.65              |
| 23:2O:54:GLY:O     | 23:2O:55:ASN:ND2   | 2.29                     | 0.65              |
| 47:2m:639:C:H2'    | 47:2m:640:A:H8     | 1.59                     | 0.65              |
| 47:2m:1595:U:H2'   | 47:2m:1596:U:H6    | 1.60                     | 0.65              |
| 47:2m:1619:A:OP1   | 57:2w:47:ARG:HD3   | 1.96                     | 0.65              |
| 47:2m:1723:G:O2'   | 47:2m:1724:A:H5'   | 1.96                     | 0.65              |
| 48:2n:34:MET:HE1   | 48:2n:162:PRO:HB3  | 1.78                     | 0.65              |
| 48:2n:56:GLU:CD    | 63:3A:79:VAL:HG12  | 2.21                     | 0.65              |
| 50:2p:60:GLY:N     | 50:2p:65:ARG:HB2   | 2.12                     | 0.65              |
| 52:2r:127:ARG:HG3  | 52:2r:137:GLN:HB2  | 1.77                     | 0.65              |
| 68:3F:44:LYS:HD3   | 68:3F:45:LEU:N     | 2.11                     | 0.65              |
| 71:3I:42:GLU:OE1   | 71:3I:42:GLU:N     | 2.29                     | 0.65              |
| 76:3N:6:THR:O      | 76:3N:7:ILE:HD13   | 1.95                     | 0.65              |
| 77:3O:47:LEU:CD2   | 77:3O:80:ARG:H     | 2.07                     | 0.65              |
| 1:1A:1077:C:O2'    | 1:1A:1078:A:H5'    | 1.97                     | 0.65              |
| 1:1A:2504:C:O2'    | 1:1A:2505:C:O5'    | 2.13                     | 0.65              |
| 11:2C:61:TRP:CH2   | 15:2G:33:GLN:HB2   | 2.32                     | 0.65              |
| 11:2C:95:VAL:HG22  | 41:2g:82:LEU:HB3   | 1.79                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:2I:185:VAL:HG23 | 17:2I:185:VAL:O    | 1.96                     | 0.65              |
| 27:2S:83:GLU:OE1   | 27:2S:83:GLU:HA    | 1.95                     | 0.65              |
| 47:2m:302:A:H1'    | 54:2t:73:THR:CG2   | 2.26                     | 0.65              |
| 47:2m:1537:A:O2'   | 47:2m:1538:C:H5'   | 1.95                     | 0.65              |
| 52:2r:125:SER:HB3  | 52:2r:203:ASN:HD21 | 1.59                     | 0.65              |
| 53:2s:100:ILE:HG13 | 53:2s:125:VAL:HG21 | 1.77                     | 0.65              |
| 66:3D:14:VAL:HG13  | 66:3D:52:GLU:HG2   | 1.77                     | 0.65              |
| 73:3K:41:ALA:HB2   | 73:3K:75:LEU:HD11  | 1.77                     | 0.65              |
| 1:1A:138:G:H2'     | 1:1A:139:G:H8      | 1.61                     | 0.65              |
| 1:1A:1913:C:O2'    | 1:1A:1914:C:H5'    | 1.97                     | 0.65              |
| 1:1A:2101:C:H5'    | 1:1A:2102:G:OP2    | 1.96                     | 0.65              |
| 1:1A:4644:G:O2'    | 1:1A:4645:C:H5'    | 1.97                     | 0.65              |
| 5:1E:393:LYS:O     | 5:1E:397:ILE:HG23  | 1.97                     | 0.65              |
| 9:2A:110:GLN:HG2   | 9:2A:115:ARG:CZ    | 2.26                     | 0.65              |
| 25:2Q:123:LYS:HD3  | 47:2m:322:C:OP1    | 1.96                     | 0.65              |
| 31:2W:13:SER:O     | 31:2W:17:ARG:HG3   | 1.96                     | 0.65              |
| 46:2I:48:ARG:HD3   | 46:2I:49:PHE:N     | 2.12                     | 0.65              |
| 47:2m:158:A:H2'    | 47:2m:159:A:O4'    | 1.97                     | 0.65              |
| 47:2m:162:C:OP1    | 70:3H:87:ARG:NH2   | 2.29                     | 0.65              |
| 47:2m:1380:C:H2'   | 47:2m:1381:G:C8    | 2.31                     | 0.65              |
| 48:2n:187:GLY:HA2  | 63:3A:45:ARG:HE    | 1.61                     | 0.65              |
| 57:2w:15:PHE:CZ    | 57:2w:109:PRO:HB2  | 2.32                     | 0.65              |
| 57:2w:85:ILE:HD11  | 57:2w:116:LEU:HA   | 1.79                     | 0.65              |
| 59:2y:36:GLU:HB3   | 59:2y:47:ARG:CD    | 2.25                     | 0.65              |
| 66:3D:31:ARG:HB2   | 66:3D:43:ILE:HD13  | 1.78                     | 0.65              |
| 1:1A:727:C:O2'     | 1:1A:728:U:H5'     | 1.97                     | 0.65              |
| 1:1A:1342:A:OP1    | 16:2H:204:ARG:HD2  | 1.96                     | 0.65              |
| 1:1A:1355:G:H2'    | 1:1A:1356:U:C6     | 2.31                     | 0.65              |
| 1:1A:1801:A:O2'    | 1:1A:1802:A:H5'    | 1.97                     | 0.65              |
| 1:1A:1949:U:O2'    | 1:1A:1950:U:H5'    | 1.97                     | 0.65              |
| 1:1A:2586:G:N3     | 1:1A:2586:G:H2'    | 2.12                     | 0.65              |
| 1:1A:4188:U:H2'    | 1:1A:4189:U:C6     | 2.32                     | 0.65              |
| 1:1A:4403:U:O2'    | 1:1A:4404:U:H5'    | 1.97                     | 0.65              |
| 1:1A:4986:G:H5''   | 5:1E:176:LYS:HG3   | 1.78                     | 0.65              |
| 32:2X:65:ASP:OD2   | 32:2X:67:ARG:HB2   | 1.97                     | 0.65              |
| 37:2c:26:HIS:O     | 37:2c:29:ARG:HG3   | 1.97                     | 0.65              |
| 47:2m:1445:U:H2'   | 47:2m:1446:A:C8    | 2.32                     | 0.65              |
| 47:2m:1486:A:O2'   | 47:2m:1487:A:OP1   | 2.14                     | 0.65              |
| 52:2r:87:LEU:HD11  | 58:2x:47:LEU:HD21  | 1.77                     | 0.65              |
| 54:2t:172:LEU:HD11 | 54:2t:195:LEU:CD1  | 2.25                     | 0.65              |
| 56:2v:37:TYR:HE2   | 56:2v:51:ILE:HG23  | 1.62                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:3B:128:VAL:HG11 | 64:3B:133:LEU:HD21 | 1.78                     | 0.65              |
| 68:3F:15:ASN:HA    | 68:3F:305:ASN:ND2  | 2.12                     | 0.65              |
| 70:3H:67:VAL:HG12  | 70:3H:69:THR:HG22  | 1.78                     | 0.65              |
| 71:3I:55:LYS:O     | 71:3I:59:GLU:HG2   | 1.96                     | 0.65              |
| 1:1A:2014:C:C4     | 1:1A:2015:U:H1'    | 2.31                     | 0.65              |
| 1:1A:4088:C:H2'    | 1:1A:4089:G:H8     | 1.62                     | 0.65              |
| 1:1A:4342:C:O3'    | 43:2i:37:GLY:HA3   | 1.97                     | 0.65              |
| 1:1A:4993:G:N1     | 1:1A:5058:A:C2     | 2.54                     | 0.65              |
| 2:1B:58:A:H2'      | 2:1B:59:G:C8       | 2.32                     | 0.65              |
| 12:2D:36:LEU:HD11  | 12:2D:69:ARG:HH11  | 1.61                     | 0.65              |
| 21:2M:15:ARG:HB3   | 21:2M:27:LEU:HD23  | 1.78                     | 0.65              |
| 47:2m:65:C:C6      | 70:3H:174:PRO:HB3  | 2.32                     | 0.65              |
| 49:2o:92:GLN:HG2   | 49:2o:97:LEU:HD11  | 1.78                     | 0.65              |
| 57:2w:25:LEU:HA    | 57:2w:28:MET:CE    | 2.27                     | 0.65              |
| 65:3C:46:GLU:N     | 65:3C:46:GLU:OE1   | 2.30                     | 0.65              |
| 67:3E:53:ILE:HD12  | 67:3E:55:LEU:HD11  | 1.78                     | 0.65              |
| 69:3G:208:PRO:O    | 69:3G:212:LYS:HG2  | 1.96                     | 0.65              |
| 71:3I:78:LEU:CD2   | 71:3I:97:ILE:HD11  | 2.27                     | 0.65              |
| 74:3L:65:ASP:O     | 74:3L:65:ASP:OD1   | 2.15                     | 0.65              |
| 1:1A:738:C:O2'     | 15:2G:71:LYS:NZ    | 2.29                     | 0.65              |
| 1:1A:3762:U:H2'    | 1:1A:3763:A:C8     | 2.32                     | 0.65              |
| 1:1A:4877:G:H1     | 21:2M:161:ARG:HH12 | 1.44                     | 0.65              |
| 13:2E:67:LYS:O     | 13:2E:68:ILE:HD13  | 1.96                     | 0.65              |
| 46:2l:39:LYS:O     | 46:2l:198:TRP:HB2  | 1.96                     | 0.65              |
| 46:2l:66:CYS:HB3   | 46:2l:82:ILE:CD1   | 2.26                     | 0.65              |
| 47:2m:321:C:H3'    | 47:2m:322:C:C6     | 2.32                     | 0.65              |
| 47:2m:612:U:H2'    | 47:2m:613:G:H5'    | 1.78                     | 0.65              |
| 47:2m:751:G:H3'    | 47:2m:752:G:O4'    | 1.96                     | 0.65              |
| 47:2m:1130:G:C2'   | 47:2m:1131:G:H5''  | 2.25                     | 0.65              |
| 47:2m:1284:A:N6    | 72:3J:91:LEU:HD21  | 2.11                     | 0.65              |
| 47:2m:1362:U:H5''  | 47:2m:1363:C:H5    | 1.61                     | 0.65              |
| 47:2m:1503:C:H2'   | 47:2m:1504:U:C6    | 2.31                     | 0.65              |
| 48:2n:218:ALA:O    | 48:2n:222:VAL:HG23 | 1.96                     | 0.65              |
| 77:3O:47:LEU:CD2   | 77:3O:83:LEU:HB2   | 2.24                     | 0.65              |
| 1:1A:126:C:H2'     | 1:1A:127:G:H8      | 1.61                     | 0.65              |
| 1:1A:2020:U:H2'    | 1:1A:2021:G:H5''   | 1.79                     | 0.65              |
| 1:1A:2670:C:O2'    | 1:1A:2671:C:H5'    | 1.97                     | 0.65              |
| 1:1A:3848:U:H2'    | 1:1A:3849:A:H8     | 1.62                     | 0.65              |
| 9:2A:25:PHE:HA     | 9:2A:28:LEU:HD11   | 1.79                     | 0.65              |
| 30:2V:23:LYS:HG3   | 30:2V:24:PRO:CD    | 2.17                     | 0.65              |
| 47:2m:1016:U:H5'   | 73:3K:15:ALA:O     | 1.96                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1402:A:H4'   | 62:21:51:LYS:HE2   | 1.79                     | 0.65              |
| 47:2m:1822:A:H2'   | 47:2m:1823:A:H8    | 1.58                     | 0.65              |
| 58:2x:29:ASN:HA    | 58:2x:64:ALA:O     | 1.97                     | 0.65              |
| 68:3F:22:ALA:CB    | 68:3F:71:ILE:HD13  | 2.27                     | 0.65              |
| 1:1A:1721:G:H2'    | 1:1A:1722:C:H6     | 1.61                     | 0.65              |
| 8:1H:50:LEU:H      | 8:1H:50:LEU:HD23   | 1.60                     | 0.65              |
| 20:2L:163:ARG:O    | 20:2L:166:THR:HG22 | 1.97                     | 0.65              |
| 47:2m:186:C:H2'    | 47:2m:187:G:C8     | 2.32                     | 0.65              |
| 47:2m:442:C:O2'    | 47:2m:443:U:H5'    | 1.97                     | 0.65              |
| 47:2m:1373:C:O2'   | 59:2y:10:LYS:HE3   | 1.97                     | 0.65              |
| 47:2m:1534:C:H5''  | 47:2m:1536:G:C1'   | 2.27                     | 0.65              |
| 49:2o:196:ASP:HA   | 49:2o:199:LYS:HZ2  | 1.60                     | 0.65              |
| 59:2y:24:LEU:HD21  | 59:2y:58:MET:HE2   | 1.78                     | 0.65              |
| 67:3E:13:LYS:HA    | 67:3E:13:LYS:HE3   | 1.78                     | 0.65              |
| 68:3F:17:TRP:HB2   | 68:3F:36:ARG:CD    | 2.23                     | 0.65              |
| 72:3J:82:ASN:O     | 72:3J:105:GLY:HA3  | 1.97                     | 0.65              |
| 77:3O:77:LEU:CD1   | 77:3O:78:LYS:H     | 2.10                     | 0.65              |
| 1:1A:1846:G:H2'    | 1:1A:1847:C:C6     | 2.31                     | 0.64              |
| 1:1A:3910:C:H2'    | 1:1A:3911:C:H6     | 1.62                     | 0.64              |
| 14:2F:87:HIS:CE1   | 14:2F:89:LYS:HG3   | 2.32                     | 0.64              |
| 20:2L:112:SER:OG   | 20:2L:114:LYS:HG3  | 1.96                     | 0.64              |
| 30:2V:105:GLY:O    | 30:2V:109:ARG:HG2  | 1.97                     | 0.64              |
| 47:2m:628:A:N6     | 50:2p:145:GLN:OE1  | 2.30                     | 0.64              |
| 47:2m:744:G:H2'    | 47:2m:744:G:N3     | 2.12                     | 0.64              |
| 47:2m:884:C:O2'    | 47:2m:885:U:H5'    | 1.97                     | 0.64              |
| 60:2z:70:ILE:HG22  | 60:2z:77:TYR:HD2   | 1.61                     | 0.64              |
| 68:3F:22:ALA:HB1   | 68:3F:71:ILE:HD13  | 1.78                     | 0.64              |
| 80:3R:137:ASP:OD1  | 80:3R:138:ARG:N    | 2.30                     | 0.64              |
| 1:1A:1081:C:H1'    | 1:1A:1219:G:H1     | 1.63                     | 0.64              |
| 1:1A:1179:U:C3'    | 1:1A:1180:C:H5''   | 2.27                     | 0.64              |
| 1:1A:1267:C:O2'    | 1:1A:1268:G:H5'    | 1.97                     | 0.64              |
| 1:1A:4056:A:N3     | 1:1A:4057:C:N4     | 2.40                     | 0.64              |
| 6:1F:209:ILE:HB    | 6:1F:229:LEU:CD1   | 2.28                     | 0.64              |
| 7:1G:39:GLN:NE2    | 7:1G:46:THR:O      | 2.27                     | 0.64              |
| 39:2e:9:LYS:HG3    | 39:2e:10:ASP:N     | 2.12                     | 0.64              |
| 47:2m:90:G:H2'     | 47:2m:91:A:O4'     | 1.98                     | 0.64              |
| 58:2x:15:ARG:CG    | 58:2x:20:THR:HG23  | 2.23                     | 0.64              |
| 64:3B:87:ASN:HB2   | 64:3B:90:CYS:HB2   | 1.78                     | 0.64              |
| 68:3F:291:TRP:CZ3  | 68:3F:298:LEU:HG   | 2.33                     | 0.64              |
| 69:3G:137:VAL:HG21 | 69:3G:217:ALA:HB2  | 1.79                     | 0.64              |
| 1:1A:453:G:H2'     | 1:1A:453:G:N3      | 2.11                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1564:A:H2'    | 1:1A:1565:A:C8     | 2.32                     | 0.64              |
| 1:1A:2092:G:O2'    | 1:1A:2093:A:OP2    | 2.13                     | 0.64              |
| 1:1A:2104:G:N3     | 1:1A:2104:G:H2'    | 2.12                     | 0.64              |
| 1:1A:2334:C:C5     | 6:1F:191:ALA:HB2   | 2.32                     | 0.64              |
| 1:1A:4870:G:OP2    | 1:1A:4870:G:N2     | 2.29                     | 0.64              |
| 14:2F:33:ILE:HG22  | 14:2F:37:LYS:NZ    | 2.12                     | 0.64              |
| 37:2c:63:VAL:CG2   | 37:2c:65:LYS:HG3   | 2.25                     | 0.64              |
| 46:2l:120:ILE:HA   | 46:2l:124:LEU:HD13 | 1.80                     | 0.64              |
| 47:2m:835:C:H42    | 76:3N:9:THR:HG22   | 1.61                     | 0.64              |
| 49:2o:92:GLN:CG    | 49:2o:97:LEU:HD11  | 2.27                     | 0.64              |
| 49:2o:98:THR:O     | 49:2o:232:HIS:NE2  | 2.28                     | 0.64              |
| 49:2o:110:MET:HA   | 49:2o:113:MET:HE2  | 1.78                     | 0.64              |
| 52:2r:47:LYS:HA    | 58:2x:115:TYR:OH   | 1.96                     | 0.64              |
| 57:2w:41:GLN:OE1   | 57:2w:84:ILE:HG12  | 1.98                     | 0.64              |
| 58:2x:50:LYS:HA    | 58:2x:53:GLU:HG3   | 1.78                     | 0.64              |
| 68:3F:79:LEU:HD21  | 68:3F:87:LEU:HD22  | 1.77                     | 0.64              |
| 68:3F:242:SER:HA   | 68:3F:291:TRP:CD1  | 2.32                     | 0.64              |
| 70:3H:113:ILE:HD12 | 70:3H:124:LEU:HD21 | 1.79                     | 0.64              |
| 73:3K:63:VAL:HA    | 73:3K:66:VAL:HG12  | 1.78                     | 0.64              |
| 73:3K:102:LEU:HD21 | 73:3K:111:ALA:CB   | 2.27                     | 0.64              |
| 78:3P:49:HIS:ND1   | 78:3P:69:GLY:O     | 2.30                     | 0.64              |
| 1:1A:3975:C:OP1    | 46:2l:26:ARG:HD3   | 1.97                     | 0.64              |
| 1:1A:4178:A:H2'    | 1:1A:4179:G:H8     | 1.62                     | 0.64              |
| 1:1A:4269:G:O2'    | 1:1A:4270:C:H5'    | 1.97                     | 0.64              |
| 1:1A:5015:G:H2'    | 1:1A:5016:A:H2     | 1.63                     | 0.64              |
| 3:1C:127:U:H2'     | 3:1C:128:C:C6      | 2.31                     | 0.64              |
| 12:2D:181:PHE:O    | 12:2D:185:VAL:HG23 | 1.97                     | 0.64              |
| 25:2Q:74:ARG:NH1   | 47:2m:1749:G:OP1   | 2.31                     | 0.64              |
| 47:2m:811:A:O2'    | 47:2m:812:A:OP1    | 2.12                     | 0.64              |
| 47:2m:1560:U:H4'   | 47:2m:1583:C:O2'   | 1.98                     | 0.64              |
| 47:2m:1589:A:H1'   | 47:2m:1653:U:O2'   | 1.97                     | 0.64              |
| 49:2o:63:LYS:HE2   | 49:2o:90:ASP:HA    | 1.78                     | 0.64              |
| 50:2p:175:VAL:HG21 | 50:2p:184:ILE:HD11 | 1.79                     | 0.64              |
| 51:2q:42:LEU:HD13  | 51:2q:109:PHE:HD2  | 1.62                     | 0.64              |
| 56:2v:40:ILE:HD12  | 56:2v:143:LEU:CD2  | 2.27                     | 0.64              |
| 66:3D:42:ILE:HG23  | 66:3D:44:ARG:HG2   | 1.79                     | 0.64              |
| 68:3F:129:ILE:HG21 | 68:3F:177:TRP:HZ3  | 1.62                     | 0.64              |
| 1:1A:65:A:C2       | 1:1A:76:A:H5''     | 2.31                     | 0.64              |
| 1:1A:1904:G:O2'    | 1:1A:1905:U:H5'    | 1.97                     | 0.64              |
| 1:1A:2034:G:H2'    | 1:1A:2035:C:C6     | 2.32                     | 0.64              |
| 1:1A:4098:A:H2'    | 1:1A:4099:G:H5'    | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4178:A:H2'    | 1:1A:4179:G:C8     | 2.32                     | 0.64              |
| 1:1A:5003:U:H2'    | 1:1A:5004:C:C6     | 2.33                     | 0.64              |
| 9:2A:28:LEU:H      | 9:2A:28:LEU:HD12   | 1.61                     | 0.64              |
| 20:2L:172:ARG:O    | 20:2L:176:ARG:HG3  | 1.98                     | 0.64              |
| 47:2m:606:G:H1'    | 79:3Q:58:ASN:OD1   | 1.97                     | 0.64              |
| 47:2m:1289:U:H5    | 80:3R:97:LYS:HE2   | 1.63                     | 0.64              |
| 47:2m:1415:C:OP2   | 47:2m:1416:C:H4'   | 1.97                     | 0.64              |
| 52:2r:195:GLU:HG3  | 52:2r:198:ARG:NH2  | 2.13                     | 0.64              |
| 58:2x:85:ARG:NH1   | 58:2x:116:ASP:OD2  | 2.30                     | 0.64              |
| 60:2z:112:GLU:HA   | 60:2z:115:LYS:HG2  | 1.80                     | 0.64              |
| 1:1A:2067:C:O2'    | 1:1A:2068:C:H5'    | 1.97                     | 0.64              |
| 1:1A:2695:A:H1'    | 1:1A:2696:A:OP2    | 1.98                     | 0.64              |
| 4:1D:118:GLU:HG3   | 4:1D:126:LEU:HD21  | 1.78                     | 0.64              |
| 6:1F:25:PRO:HG2    | 6:1F:28:PHE:CD2    | 2.33                     | 0.64              |
| 25:2Q:78:PHE:CE2   | 70:3H:8:PRO:HB2    | 2.31                     | 0.64              |
| 47:2m:850:C:O2'    | 47:2m:851:C:OP1    | 2.16                     | 0.64              |
| 47:2m:1036:A:H4'   | 47:2m:1855:G:N2    | 2.12                     | 0.64              |
| 47:2m:1348:G:N2    | 47:2m:1381:G:H22   | 1.96                     | 0.64              |
| 47:2m:1612:G:O2'   | 47:2m:1613:G:H5'   | 1.96                     | 0.64              |
| 50:2p:29:LEU:HD12  | 50:2p:29:LEU:H     | 1.61                     | 0.64              |
| 54:2t:151:GLU:HA   | 54:2t:154:LYS:CE   | 2.21                     | 0.64              |
| 57:2w:111:MET:HB3  | 60:2z:117:ILE:CD1  | 2.27                     | 0.64              |
| 62:21:40:ILE:O     | 62:21:44:LYS:HG2   | 1.97                     | 0.64              |
| 62:21:41:ARG:HA    | 62:21:44:LYS:CE    | 2.27                     | 0.64              |
| 66:3D:30:VAL:HG22  | 66:3D:44:ARG:O     | 1.97                     | 0.64              |
| 68:3F:194:TYR:CE1  | 68:3F:212:LYS:HB2  | 2.33                     | 0.64              |
| 68:3F:289:LEU:HD11 | 68:3F:298:LEU:HD22 | 1.79                     | 0.64              |
| 74:3L:45:THR:OG1   | 74:3L:49:GLY:HA2   | 1.98                     | 0.64              |
| 75:3M:84:LYS:H     | 75:3M:84:LYS:HD2   | 1.61                     | 0.64              |
| 1:1A:1670:G:O2'    | 1:1A:1853:G:H4'    | 1.96                     | 0.64              |
| 1:1A:4892:A:H61    | 1:1A:4928:C:H42    | 1.44                     | 0.64              |
| 5:1E:391:PRO:HD2   | 25:2Q:63:GLN:OE1   | 1.98                     | 0.64              |
| 12:2D:38:ARG:NH2   | 12:2D:45:GLU:OE1   | 2.27                     | 0.64              |
| 26:2R:56:ARG:O     | 26:2R:57:GLN:NE2   | 2.31                     | 0.64              |
| 35:2a:82:MET:HE1   | 35:2a:90:ARG:HD3   | 1.80                     | 0.64              |
| 47:2m:566:U:H3     | 47:2m:584:G:H1     | 1.46                     | 0.64              |
| 47:2m:579:C:O2'    | 47:2m:580:U:OP1    | 2.14                     | 0.64              |
| 47:2m:1123:C:O2'   | 49:2o:148:ASN:OD1  | 2.15                     | 0.64              |
| 51:2q:212:ASP:OD1  | 51:2q:214:ASN:N    | 2.25                     | 0.64              |
| 58:2x:23:ALA:CB    | 58:2x:70:VAL:HG22  | 2.28                     | 0.64              |
| 58:2x:39:LEU:O     | 58:2x:42:ILE:HB    | 1.97                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:2x:110:ASP:OD1  | 58:2x:111:ILE:N    | 2.30                     | 0.64              |
| 60:2z:25:LYS:HA    | 60:2z:55:ARG:HA    | 1.78                     | 0.64              |
| 68:3F:306:LEU:HD12 | 68:3F:307:VAL:N    | 2.12                     | 0.64              |
| 70:3H:195:LYS:HG3  | 70:3H:198:ARG:NH2  | 2.12                     | 0.64              |
| 80:3R:135:HIS:NE2  | 80:3R:140:TYR:HB3  | 2.13                     | 0.64              |
| 1:1A:397:G:C2'     | 1:1A:398:A:H5'     | 2.27                     | 0.64              |
| 1:1A:4579:U:O2'    | 1:1A:4580:U:H5'    | 1.98                     | 0.64              |
| 9:2A:127:LYS:HB2   | 22:2N:133:ALA:HB3  | 1.79                     | 0.64              |
| 10:2B:77:PRO:HG2   | 10:2B:80:ILE:HD12  | 1.79                     | 0.64              |
| 10:2B:256:ALA:O    | 10:2B:259:LYS:HG2  | 1.98                     | 0.64              |
| 46:2l:120:ILE:HA   | 46:2l:124:LEU:CD1  | 2.27                     | 0.64              |
| 48:2n:18:PHE:CE1   | 48:2n:177:MET:HE1  | 2.33                     | 0.64              |
| 51:2q:252:ARG:O    | 51:2q:256:LEU:HG   | 1.98                     | 0.64              |
| 60:2z:132:ARG:O    | 60:2z:134:GLN:NE2  | 2.31                     | 0.64              |
| 66:3D:11:LEU:HD12  | 66:3D:55:VAL:HG22  | 1.78                     | 0.64              |
| 70:3H:16:ILE:HD12  | 70:3H:17:GLU:H     | 1.62                     | 0.64              |
| 70:3H:23:LYS:HE3   | 70:3H:42:GLY:H     | 1.62                     | 0.64              |
| 71:3l:67:ASP:OD1   | 71:3l:70:ARG:N     | 2.29                     | 0.64              |
| 1:1A:264:C:H4'     | 1:1A:265:C:OP1     | 1.97                     | 0.64              |
| 1:1A:369:G:N2      | 1:1A:372:A:OP2     | 2.27                     | 0.64              |
| 1:1A:1065:G:H2'    | 1:1A:1066:G:O4'    | 1.98                     | 0.64              |
| 1:1A:1196:G:H2'    | 1:1A:1197:C:C6     | 2.32                     | 0.64              |
| 1:1A:2005:G:H2'    | 1:1A:2006:U:C5     | 2.29                     | 0.64              |
| 1:1A:2807:A:O4'    | 35:2a:2:VAL:HG11   | 1.98                     | 0.64              |
| 1:1A:2815:A:H2'    | 1:1A:2816:G:H8     | 1.60                     | 0.64              |
| 1:1A:3783:A:H2     | 1:1A:3790:U:H3     | 1.45                     | 0.64              |
| 1:1A:4252:C:OP2    | 1:1A:4253:A:O2'    | 2.04                     | 0.64              |
| 12:2D:200:VAL:HG13 | 12:2D:208:LYS:HZ2  | 1.62                     | 0.64              |
| 13:2E:90:ARG:C     | 13:2E:91:GLU:HG3   | 2.22                     | 0.64              |
| 25:2Q:98:PRO:O     | 25:2Q:100:VAL:HG23 | 1.97                     | 0.64              |
| 47:2m:551:U:H5''   | 47:2m:552:G:OP2    | 1.98                     | 0.64              |
| 47:2m:1622:U:H4'   | 47:2m:1623:A:OP2   | 1.98                     | 0.64              |
| 47:2m:1818:A:H2'   | 47:2m:1819:A:H5''  | 1.79                     | 0.64              |
| 50:2p:135:GLU:CG   | 50:2p:153:VAL:HB   | 2.21                     | 0.64              |
| 53:2s:148:LEU:N    | 75:3M:49:GLU:OE2   | 2.30                     | 0.64              |
| 54:2t:56:ARG:CB    | 54:2t:180:GLY:HA2  | 2.28                     | 0.64              |
| 55:2u:35:LEU:HD21  | 55:2u:38:LYS:H     | 1.63                     | 0.64              |
| 59:2y:71:ILE:H     | 59:2y:71:ILE:HD12  | 1.62                     | 0.64              |
| 68:3F:254:PRO:HG3  | 68:3F:283:PRO:HB2  | 1.78                     | 0.64              |
| 73:3K:93:LYS:HB2   | 73:3K:150:VAL:HG21 | 1.79                     | 0.64              |
| 76:3N:50:THR:HG21  | 76:3N:75:ILE:HD11  | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:3Q:28:LYS:HB3   | 79:3Q:32:ALA:HB3   | 1.80                     | 0.64              |
| 1:1A:186:G:O6      | 1:1A:1365:C:H4'    | 1.98                     | 0.64              |
| 1:1A:453:G:H4'     | 1:1A:454:U:H5'     | 1.80                     | 0.64              |
| 1:1A:485:C:O2      | 1:1A:485:C:H2'     | 1.97                     | 0.64              |
| 1:1A:683:C:H2'     | 1:1A:684:G:O4'     | 1.98                     | 0.64              |
| 1:1A:1366:G:C2'    | 1:1A:1367:C:H5''   | 2.27                     | 0.64              |
| 1:1A:4413:C:H5     | 1:1A:4429:C:H42    | 1.45                     | 0.64              |
| 10:2B:108:GLN:OE1  | 10:2B:108:GLN:N    | 2.29                     | 0.64              |
| 10:2B:250:ILE:O    | 10:2B:254:GLU:HG3  | 1.98                     | 0.64              |
| 23:2O:24:ASP:OD2   | 23:2O:69:LYS:NZ    | 2.30                     | 0.64              |
| 47:2m:138:C:H5''   | 47:2m:139:C:C5     | 2.31                     | 0.64              |
| 47:2m:888:U:O2     | 47:2m:889:U:H2'    | 1.98                     | 0.64              |
| 47:2m:996:A:H5''   | 73:3K:7:PRO:HG3    | 1.79                     | 0.64              |
| 47:2m:1282:A:H2'   | 47:2m:1282:A:N3    | 2.13                     | 0.64              |
| 47:2m:1617:G:H2'   | 47:2m:1619:A:OP2   | 1.98                     | 0.64              |
| 48:2n:170:SER:O    | 48:2n:174:MET:HE2  | 1.98                     | 0.64              |
| 53:2s:181:THR:HG22 | 53:2s:183:LYS:HG3  | 1.80                     | 0.64              |
| 54:2t:165:GLN:HB2  | 54:2t:171:LEU:HD23 | 1.80                     | 0.64              |
| 57:2w:80:LEU:O     | 57:2w:116:LEU:HD21 | 1.98                     | 0.64              |
| 61:20:110:LEU:HD22 | 61:20:112:MET:HE3  | 1.80                     | 0.64              |
| 68:3F:225:LYS:HG3  | 68:3F:226:HIS:N    | 2.13                     | 0.64              |
| 76:3N:22:GLN:CD    | 76:3N:74:MET:HE1   | 2.23                     | 0.64              |
| 1:1A:265:C:H1'     | 36:2b:112:ARG:HH22 | 1.63                     | 0.63              |
| 1:1A:452:A:O2'     | 8:1H:224:LYS:HD3   | 1.98                     | 0.63              |
| 1:1A:992:C:H2'     | 1:1A:993:G:H5'     | 1.80                     | 0.63              |
| 1:1A:1328:G:O2'    | 1:1A:2349:A:OP1    | 2.16                     | 0.63              |
| 1:1A:1363:C:H3'    | 14:2F:36:ARG:NH2   | 2.12                     | 0.63              |
| 1:1A:1890:G:N2     | 1:1A:1890:G:OP2    | 2.31                     | 0.63              |
| 1:1A:2257:C:O2     | 1:1A:2257:C:H2'    | 1.99                     | 0.63              |
| 1:1A:2711:G:OP2    | 1:1A:2712:G:H5''   | 1.97                     | 0.63              |
| 1:1A:4247:G:O2'    | 1:1A:4248:A:H5'    | 1.98                     | 0.63              |
| 14:2F:51:ALA:HB2   | 14:2F:149:GLN:NE2  | 2.13                     | 0.63              |
| 14:2F:63:THR:CG2   | 14:2F:65:ARG:H     | 2.10                     | 0.63              |
| 42:2h:12:ARG:HG2   | 42:2h:15:ARG:HH21  | 1.62                     | 0.63              |
| 46:2l:65:VAL:HG22  | 46:2l:109:ALA:O    | 1.98                     | 0.63              |
| 46:2l:73:HIS:NE2   | 46:2l:111:LEU:HD21 | 2.12                     | 0.63              |
| 46:2l:95:LYS:HB3   | 46:2l:104:ALA:CB   | 2.28                     | 0.63              |
| 47:2m:127:C:N4     | 47:2m:181:A:O2'    | 2.31                     | 0.63              |
| 47:2m:311:C:H2'    | 47:2m:312:G:C1'    | 2.29                     | 0.63              |
| 47:2m:396:U:H4'    | 54:2t:14:THR:HG22  | 1.79                     | 0.63              |
| 47:2m:1005:G:H2'   | 47:2m:1006:C:H6    | 1.63                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1620:A:H4'   | 47:2m:1621:U:C5    | 2.33                     | 0.63              |
| 51:2q:37:LYS:O     | 51:2q:41:CYS:HB3   | 1.98                     | 0.63              |
| 53:2s:19:PHE:O     | 53:2s:23:ILE:HD11  | 1.98                     | 0.63              |
| 55:2u:25:LYS:CD    | 55:2u:46:MET:HE1   | 2.12                     | 0.63              |
| 57:2w:70:MET:H     | 57:2w:70:MET:HE3   | 1.63                     | 0.63              |
| 60:2z:23:ARG:HB3   | 77:3O:48:VAL:CG1   | 2.28                     | 0.63              |
| 63:3A:25:GLY:O     | 69:3G:85:SER:OG    | 2.15                     | 0.63              |
| 76:3N:6:THR:CG2    | 76:3N:28:LEU:HB2   | 2.24                     | 0.63              |
| 1:1A:3670:C:O2'    | 1:1A:3671:G:H8     | 1.81                     | 0.63              |
| 1:1A:5014:A:O2'    | 1:1A:5015:G:H5'    | 1.98                     | 0.63              |
| 8:1H:112:MET:HE3   | 45:2k:94:ARG:NH1   | 2.14                     | 0.63              |
| 13:2E:9:GLU:HB2    | 13:2E:13:ARG:HB2   | 1.80                     | 0.63              |
| 18:2J:94:MET:HG2   | 18:2J:148:MET:CE   | 2.27                     | 0.63              |
| 36:2b:32:ARG:HG2   | 36:2b:32:ARG:HH11  | 1.63                     | 0.63              |
| 47:2m:126:G:OP2    | 70:3H:195:LYS:HG2  | 1.98                     | 0.63              |
| 47:2m:642:U:H5''   | 71:3I:41:ARG:NH1   | 2.13                     | 0.63              |
| 47:2m:863:U:OP1    | 75:3M:32:LYS:HE3   | 1.98                     | 0.63              |
| 81:2m:1902:84D:N2  | 81:2m:1902:84D:O7  | 2.31                     | 0.63              |
| 52:2r:20:PHE:HE2   | 52:2r:94:LYS:HB2   | 1.61                     | 0.63              |
| 53:2s:15:LYS:H     | 53:2s:16:PRO:HD2   | 1.61                     | 0.63              |
| 58:2x:39:LEU:HB3   | 58:2x:51:LEU:CD2   | 2.28                     | 0.63              |
| 60:2z:40:TYR:CZ    | 60:2z:97:GLN:HG2   | 2.33                     | 0.63              |
| 61:20:14:PHE:CD1   | 61:20:134:ILE:HD11 | 2.32                     | 0.63              |
| 73:3K:87:ASP:OD1   | 73:3K:87:ASP:N     | 2.28                     | 0.63              |
| 1:1A:180:C:H2'     | 1:1A:181:C:C6      | 2.34                     | 0.63              |
| 1:1A:209:U:H2'     | 1:1A:210:C:H2'     | 1.81                     | 0.63              |
| 1:1A:1480:C:O2'    | 1:1A:1482:G:OP2    | 2.14                     | 0.63              |
| 1:1A:1693:U:P      | 19:2K:53:MET:HE1   | 2.38                     | 0.63              |
| 1:1A:1824:G:H2'    | 1:1A:1825:A:C8     | 2.33                     | 0.63              |
| 1:1A:3944:G:O3'    | 49:2o:54:GLY:HA2   | 1.98                     | 0.63              |
| 1:1A:3974:G:H22    | 1:1A:4050:A:H3'    | 1.61                     | 0.63              |
| 1:1A:4108:G:H4'    | 1:1A:4109:G:OP1    | 1.97                     | 0.63              |
| 1:1A:4111:U:H2'    | 1:1A:4112:C:H1'    | 1.81                     | 0.63              |
| 1:1A:4486:C:H2'    | 1:1A:4487:A:O4'    | 1.98                     | 0.63              |
| 1:1A:4759:C:H2'    | 1:1A:4760:G:O4'    | 1.96                     | 0.63              |
| 1:1A:4904:G:O2'    | 1:1A:4905:C:H5'    | 1.99                     | 0.63              |
| 5:1E:303:ALA:HB3   | 5:1E:312:LYS:O     | 1.98                     | 0.63              |
| 25:2Q:101:ARG:HD3  | 25:2Q:105:ARG:NH2  | 2.13                     | 0.63              |
| 28:2T:36:ARG:NH1   | 28:2T:38:TYR:OH    | 2.31                     | 0.63              |
| 29:2U:103:VAL:HG23 | 29:2U:108:TYR:O    | 1.98                     | 0.63              |
| 35:2a:60:ARG:O     | 35:2a:63:VAL:HG13  | 1.98                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:2i:99:ARG:HD3   | 43:2i:100:LYS:H    | 1.62                     | 0.63              |
| 47:2m:170:A:OP1    | 70:3H:136:LYS:N    | 2.21                     | 0.63              |
| 47:2m:1148:A:H4'   | 47:2m:1149:A:O4'   | 1.99                     | 0.63              |
| 47:2m:1361:G:OP2   | 47:2m:1362:U:O2'   | 2.14                     | 0.63              |
| 47:2m:1541:G:O2'   | 47:2m:1542:C:H5'   | 1.98                     | 0.63              |
| 47:2m:1619:A:OP1   | 57:2w:47:ARG:NH1   | 2.32                     | 0.63              |
| 47:2m:1831:A:H1'   | 47:2m:1852:C:OP1   | 1.98                     | 0.63              |
| 48:2n:18:PHE:CZ    | 48:2n:177:MET:HE1  | 2.34                     | 0.63              |
| 48:2n:85:ARG:NH2   | 48:2n:201:LEU:HD12 | 2.13                     | 0.63              |
| 50:2p:96:LEU:CD2   | 50:2p:198:ILE:HG23 | 2.28                     | 0.63              |
| 55:2u:15:LEU:HD13  | 55:2u:49:MET:CE    | 2.28                     | 0.63              |
| 66:3D:59:LEU:O     | 66:3D:60:GLU:HG3   | 1.98                     | 0.63              |
| 70:3H:67:VAL:HG12  | 70:3H:69:THR:CG2   | 2.27                     | 0.63              |
| 76:3N:92:ALA:HB2   | 76:3N:97:TYR:O     | 1.99                     | 0.63              |
| 77:3O:97:ILE:HG21  | 77:3O:109:TYR:HB3  | 1.79                     | 0.63              |
| 1:1A:1501:C:H2'    | 19:2K:68:ARG:NH1   | 2.14                     | 0.63              |
| 1:1A:4242:U:H3     | 1:1A:4281:A:H2     | 1.44                     | 0.63              |
| 1:1A:4323:A:H2     | 7:1G:146:LEU:HD23  | 1.62                     | 0.63              |
| 9:2A:110:GLN:NE2   | 19:2K:4:ASP:OD2    | 2.29                     | 0.63              |
| 11:2C:106:GLN:HB2  | 11:2C:111:LEU:HB3  | 1.80                     | 0.63              |
| 12:2D:101:LYS:CE   | 12:2D:103:LEU:HD13 | 2.28                     | 0.63              |
| 30:2V:102:PRO:O    | 30:2V:109:ARG:NH2  | 2.29                     | 0.63              |
| 46:2l:36:ILE:HD11  | 46:2l:165:LEU:CD1  | 2.27                     | 0.63              |
| 47:2m:1219:C:C4'   | 66:3D:24:GLN:HG2   | 2.29                     | 0.63              |
| 47:2m:1554:C:H5''  | 47:2m:1555:U:O4'   | 1.99                     | 0.63              |
| 47:2m:1654:G:O2'   | 47:2m:1655:C:H5'   | 1.97                     | 0.63              |
| 50:2p:25:LEU:CD1   | 50:2p:37:VAL:HG11  | 2.28                     | 0.63              |
| 50:2p:113:LEU:HD23 | 50:2p:118:ALA:HB2  | 1.80                     | 0.63              |
| 52:2r:40:ALA:HA    | 52:2r:45:TYR:CZ    | 2.33                     | 0.63              |
| 53:2s:31:GLU:HA    | 53:2s:37:LYS:HE3   | 1.79                     | 0.63              |
| 62:21:31:SER:O     | 62:21:35:VAL:HG23  | 1.97                     | 0.63              |
| 63:3A:47:ASN:OD1   | 63:3A:48:GLY:N     | 2.31                     | 0.63              |
| 1:1A:180:C:H2'     | 1:1A:181:C:N1      | 2.13                     | 0.63              |
| 1:1A:914:U:H1'     | 1:1A:915:A:OP2     | 1.99                     | 0.63              |
| 1:1A:1433:A:H2'    | 1:1A:1434:G:O4'    | 1.98                     | 0.63              |
| 1:1A:1653:A:H5''   | 1:1A:1654:G:OP1    | 1.98                     | 0.63              |
| 1:1A:1907:A:H5'    | 9:2A:220:MET:HE3   | 1.79                     | 0.63              |
| 1:1A:3651:A:H2'    | 1:1A:3652:A:C8     | 2.34                     | 0.63              |
| 1:1A:4133:C:O2'    | 1:1A:4134:C:H5'    | 1.97                     | 0.63              |
| 10:2B:244:PRO:O    | 10:2B:247:VAL:HG22 | 1.98                     | 0.63              |
| 18:2J:36:ILE:HD11  | 18:2J:47:TYR:HD2   | 1.61                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:2T:107:LYS:HE2  | 28:2T:111:ARG:HH12 | 1.63                     | 0.63              |
| 32:2X:43:PRO:O     | 32:2X:47:LYS:HG3   | 1.98                     | 0.63              |
| 46:2L:12:GLU:HB2   | 46:2L:216:LEU:HD12 | 1.79                     | 0.63              |
| 46:2L:54:ARG:HA    | 46:2L:154:THR:CG2  | 2.27                     | 0.63              |
| 47:2m:416:U:O2'    | 47:2m:417:C:H5'    | 1.99                     | 0.63              |
| 47:2m:1760:G:C5    | 47:2m:1761:U:H1'   | 2.33                     | 0.63              |
| 48:2n:145:ILE:CG1  | 48:2n:159:ILE:HD13 | 2.25                     | 0.63              |
| 52:2r:127:ARG:NH1  | 52:2r:128:ILE:HG13 | 2.14                     | 0.63              |
| 55:2u:16:PHE:HB2   | 55:2u:79:LEU:HD13  | 1.79                     | 0.63              |
| 55:2u:85:LEU:HD23  | 55:2u:86:PRO:O     | 1.97                     | 0.63              |
| 59:2y:73:LEU:HA    | 59:2y:76:GLU:HG2   | 1.81                     | 0.63              |
| 60:2z:63:GLU:HG2   | 60:2z:66:ARG:NH2   | 2.12                     | 0.63              |
| 68:3F:191:HIS:CD2  | 68:3F:195:LEU:HD21 | 2.33                     | 0.63              |
| 69:3G:156:ILE:HG13 | 69:3G:157:LEU:HD22 | 1.81                     | 0.63              |
| 70:3H:68:LEU:HD12  | 70:3H:68:LEU:O     | 1.99                     | 0.63              |
| 79:3Q:28:LYS:HB3   | 79:3Q:32:ALA:CB    | 2.28                     | 0.63              |
| 1:1A:126:C:H2'     | 1:1A:127:G:C8      | 2.34                     | 0.63              |
| 1:1A:379:G:O2'     | 1:1A:380:U:H5'     | 1.99                     | 0.63              |
| 1:1A:433:A:C2      | 1:1A:3867:A:H4'    | 2.34                     | 0.63              |
| 1:1A:460:C:O2'     | 1:1A:461:G:H5'     | 1.99                     | 0.63              |
| 1:1A:1748:U:O2'    | 1:1A:1749:A:H5'    | 1.97                     | 0.63              |
| 1:1A:4906:C:H2'    | 1:1A:4907:G:C8     | 2.33                     | 0.63              |
| 3:1C:19:C:H2'      | 3:1C:20:A:H8       | 1.62                     | 0.63              |
| 22:2N:157:GLU:CG   | 22:2N:159:MET:HE2  | 2.29                     | 0.63              |
| 30:2V:91:ARG:HB3   | 30:2V:94:ASP:OD1   | 1.98                     | 0.63              |
| 32:2X:19:GLU:HG3   | 32:2X:92:ARG:HH12  | 1.64                     | 0.63              |
| 32:2X:93:ASN:N     | 32:2X:101:LYS:O    | 2.20                     | 0.63              |
| 47:2m:78:C:O2'     | 70:3H:175:LYS:HE2  | 1.98                     | 0.63              |
| 64:3B:57:VAL:HG22  | 64:3B:67:ARG:HB2   | 1.80                     | 0.63              |
| 68:3F:140:TYR:OH   | 68:3F:182:CYS:HB2  | 1.99                     | 0.63              |
| 68:3F:254:PRO:HB3  | 68:3F:284:PRO:O    | 1.99                     | 0.63              |
| 70:3H:200:LYS:O    | 70:3H:204:GLU:HG3  | 1.99                     | 0.63              |
| 1:1A:7:C:H2'       | 1:1A:8:U:C6        | 2.33                     | 0.63              |
| 1:1A:271:C:H2'     | 1:1A:272:U:C6      | 2.34                     | 0.63              |
| 1:1A:2026:A:H2'    | 1:1A:2027:U:C6     | 2.34                     | 0.63              |
| 1:1A:4155:C:H2'    | 1:1A:4156:G:O4'    | 1.99                     | 0.63              |
| 7:1G:215:ASP:OD1   | 7:1G:216:GLU:N     | 2.31                     | 0.63              |
| 9:2A:25:PHE:HA     | 9:2A:28:LEU:CD1    | 2.29                     | 0.63              |
| 11:2C:59:LYS:HE3   | 11:2C:66:GLU:HB3   | 1.81                     | 0.63              |
| 14:2F:145:LYS:O    | 14:2F:145:LYS:HD3  | 1.97                     | 0.63              |
| 31:2W:11:LEU:HA    | 31:2W:14:ILE:CG2   | 2.28                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:2Y:91:CYS:O     | 33:2Y:93:LYS:N     | 2.31                     | 0.63              |
| 47:2m:642:U:H5''   | 71:3I:41:ARG:HH12  | 1.64                     | 0.63              |
| 47:2m:752:G:H4'    | 47:2m:753:C:OP1    | 1.98                     | 0.63              |
| 47:2m:1113:A:H3'   | 47:2m:1114:U:H5'   | 1.81                     | 0.63              |
| 48:2n:24:HIS:HB3   | 48:2n:51:LEU:HD21  | 1.81                     | 0.63              |
| 48:2n:66:VAL:HG21  | 48:2n:185:MET:CB   | 2.28                     | 0.63              |
| 68:3F:163:PRO:O    | 68:3F:179:LEU:HD22 | 1.99                     | 0.63              |
| 71:3I:29:LEU:HG    | 79:3Q:42:PHE:HE2   | 1.63                     | 0.63              |
| 72:3J:86:GLY:CA    | 72:3J:105:GLY:HA2  | 2.25                     | 0.63              |
| 75:3M:25:VAL:HG12  | 75:3M:63:VAL:HB    | 1.80                     | 0.63              |
| 1:1A:305:A:OP2     | 16:2H:15:GLN:NE2   | 2.31                     | 0.63              |
| 1:1A:1048:G:O2'    | 1:1A:1049:C:O4'    | 2.17                     | 0.63              |
| 1:1A:1727:U:O2'    | 1:1A:1728:U:H5'    | 1.99                     | 0.63              |
| 1:1A:1754:U:H2'    | 1:1A:1755:C:C6     | 2.34                     | 0.63              |
| 1:1A:3710:G:H5'    | 1:1A:3711:A:OP1    | 1.99                     | 0.63              |
| 1:1A:4123:C:O2'    | 1:1A:4124:G:H5'    | 1.98                     | 0.63              |
| 1:1A:4730:C:O3'    | 1:1A:4731:G:H3'    | 1.99                     | 0.63              |
| 1:1A:4905:C:H2'    | 1:1A:4906:C:H6     | 1.64                     | 0.63              |
| 2:1B:51:G:O2'      | 2:1B:52:C:H5'      | 1.98                     | 0.63              |
| 8:1H:201:ILE:HD11  | 8:1H:267:LEU:HD21  | 1.80                     | 0.63              |
| 47:2m:416:U:C2'    | 47:2m:417:C:H5'    | 2.28                     | 0.63              |
| 47:2m:969:U:C4'    | 47:2m:971:G:H1'    | 2.29                     | 0.63              |
| 47:2m:1113:A:H5'   | 47:2m:1114:U:OP2   | 1.99                     | 0.63              |
| 47:2m:1302:G:N2    | 80:3R:95:ARG:HH22  | 1.97                     | 0.63              |
| 47:2m:1535:U:O2    | 52:2r:88:MET:HE1   | 1.99                     | 0.63              |
| 47:2m:1810:U:O2'   | 47:2m:1811:C:H5'   | 1.99                     | 0.63              |
| 50:2p:99:ILE:O     | 50:2p:103:GLU:OE1  | 2.16                     | 0.63              |
| 58:2x:97:GLN:HG2   | 68:3F:60:ARG:NH1   | 2.14                     | 0.63              |
| 60:2z:50:ILE:HG23  | 60:2z:66:ARG:HH21  | 1.63                     | 0.63              |
| 68:3F:59:LEU:HD22  | 68:3F:90:TRP:CE3   | 2.34                     | 0.63              |
| 70:3H:176:ILE:HG21 | 70:3H:179:LEU:HD13 | 1.81                     | 0.63              |
| 72:3J:117:GLU:OE2  | 72:3J:120:ALA:HB3  | 1.99                     | 0.63              |
| 1:1A:1176:C:H42    | 1:1A:1184:A:H61    | 1.47                     | 0.63              |
| 1:1A:1973:G:H3'    | 1:1A:1974:U:C5'    | 2.27                     | 0.63              |
| 1:1A:2034:G:H2'    | 1:1A:2035:C:H6     | 1.64                     | 0.63              |
| 1:1A:4743:G:H2'    | 1:1A:4744:A:O4'    | 1.99                     | 0.63              |
| 1:1A:4953:G:H2'    | 1:1A:4954:G:H8     | 1.64                     | 0.63              |
| 7:1G:108:ARG:CZ    | 7:1G:253:TYR:HB2   | 2.29                     | 0.63              |
| 10:2B:190:LEU:O    | 10:2B:193:LEU:HG   | 1.98                     | 0.63              |
| 24:2P:65:VAL:HG22  | 24:2P:73:ARG:HA    | 1.81                     | 0.63              |
| 46:2L:59:PRO:HA    | 46:2L:171:HIS:O    | 1.98                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:2l:110:PHE:O   | 46:2l:135:PRO:HB3  | 1.99                     | 0.63              |
| 47:2m:216:C:H5    | 47:2m:309:G:H1     | 1.44                     | 0.63              |
| 47:2m:311:C:H2'   | 47:2m:312:G:H1'    | 1.81                     | 0.63              |
| 47:2m:465:A:H5'   | 47:2m:466:G:N7     | 2.14                     | 0.63              |
| 51:2q:43:PRO:CG   | 51:2q:46:ILE:HG12  | 2.27                     | 0.63              |
| 64:3B:128:VAL:CG1 | 64:3B:133:LEU:HD21 | 2.29                     | 0.63              |
| 68:3F:285:GLN:HB2 | 68:3F:303:THR:HG21 | 1.81                     | 0.63              |
| 69:3G:73:MET:HE1  | 69:3G:96:PHE:HZ    | 1.64                     | 0.63              |
| 70:3H:50:VAL:HG23 | 70:3H:112:VAL:C    | 2.23                     | 0.63              |
| 77:3O:47:LEU:CG   | 77:3O:83:LEU:HD12  | 2.29                     | 0.63              |
| 1:1A:1563:A:O2'   | 1:1A:1564:A:O5'    | 2.15                     | 0.62              |
| 1:1A:1726:U:H5'   | 9:2A:135:ILE:HD11  | 1.80                     | 0.62              |
| 1:1A:3670:C:H5''  | 16:2H:75:VAL:O     | 1.98                     | 0.62              |
| 1:1A:3773:U:H4'   | 1:1A:3774:A:C5'    | 2.28                     | 0.62              |
| 1:1A:4418:G:O6    | 1:1A:4421:C:H2'    | 1.98                     | 0.62              |
| 1:1A:4878:C:H2'   | 1:1A:4879:C:H6     | 1.63                     | 0.62              |
| 6:1F:25:PRO:HG2   | 6:1F:28:PHE:CE2    | 2.34                     | 0.62              |
| 16:2H:145:ASN:O   | 16:2H:148:THR:HG22 | 1.99                     | 0.62              |
| 19:2K:178:ARG:HA  | 19:2K:184:ARG:O    | 1.98                     | 0.62              |
| 47:2m:686:U:O2    | 53:2s:118:ARG:NH2  | 2.19                     | 0.62              |
| 47:2m:1004:U:H2'  | 47:2m:1005:G:H8    | 1.64                     | 0.62              |
| 47:2m:1142:G:H2'  | 47:2m:1144:A:OP2   | 1.99                     | 0.62              |
| 47:2m:1284:A:O2'  | 72:3J:106:CYS:HA   | 1.99                     | 0.62              |
| 51:2q:247:THR:N   | 51:2q:250:GLU:OE2  | 2.29                     | 0.62              |
| 53:2s:31:GLU:HB2  | 53:2s:32:MET:HE2   | 1.79                     | 0.62              |
| 53:2s:60:ILE:HD11 | 53:2s:90:LYS:HG2   | 1.80                     | 0.62              |
| 62:21:24:LEU:HD13 | 62:21:32:LEU:HD11  | 1.79                     | 0.62              |
| 77:3O:60:LYS:HG3  | 77:3O:61:GLU:CD    | 2.24                     | 0.62              |
| 1:1A:467:U:C2     | 1:1A:468:U:H1'     | 2.34                     | 0.62              |
| 1:1A:662:C:H2'    | 1:1A:663:G:C8      | 2.34                     | 0.62              |
| 1:1A:982:U:C5     | 8:1H:71:ARG:HD2    | 2.34                     | 0.62              |
| 1:1A:1743:A:O4'   | 7:1G:15:ARG:HD2    | 2.00                     | 0.62              |
| 1:1A:2412:A:H2'   | 1:1A:2413:U:C6     | 2.34                     | 0.62              |
| 1:1A:2503:G:O6    | 4:1D:72:ARG:NH1    | 2.33                     | 0.62              |
| 1:1A:2671:C:H2'   | 1:1A:2672:C:C6     | 2.34                     | 0.62              |
| 1:1A:3972:A:H4'   | 1:1A:3973:G:O5'    | 1.99                     | 0.62              |
| 1:1A:4699:U:H4'   | 1:1A:4700:A:OP1    | 1.97                     | 0.62              |
| 3:1C:87:G:O6      | 27:2S:113:LYS:NZ   | 2.30                     | 0.62              |
| 5:1E:288:GLY:HA3  | 5:1E:330:PHE:CE1   | 2.34                     | 0.62              |
| 47:2m:126:G:H4'   | 47:2m:215:G:N2     | 2.14                     | 0.62              |
| 47:2m:886:A:C2    | 47:2m:901:G:H1'    | 2.34                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:930:C:O2'    | 47:2m:931:C:H5'    | 1.99                     | 0.62              |
| 47:2m:1387:G:H22   | 50:2p:206:ASP:HB3  | 1.63                     | 0.62              |
| 47:2m:1567:G:OP1   | 47:2m:1567:G:N2    | 2.21                     | 0.62              |
| 51:2q:43:PRO:O     | 51:2q:46:ILE:HG13  | 1.99                     | 0.62              |
| 51:2q:147:ILE:HG21 | 51:2q:169:ILE:CD1  | 2.29                     | 0.62              |
| 52:2r:42:LYS:H     | 52:2r:45:TYR:HE1   | 1.47                     | 0.62              |
| 52:2r:56:TYR:HE1   | 52:2r:65:GLN:HG3   | 1.64                     | 0.62              |
| 52:2r:82:ASN:HB2   | 52:2r:85:LYS:HD2   | 1.81                     | 0.62              |
| 56:2v:49:GLU:OE1   | 56:2v:49:GLU:N     | 2.28                     | 0.62              |
| 57:2w:111:MET:HB3  | 60:2z:117:ILE:HG12 | 1.81                     | 0.62              |
| 58:2x:61:GLU:OE1   | 58:2x:61:GLU:N     | 2.31                     | 0.62              |
| 76:3N:45:ALA:HB1   | 76:3N:50:THR:O     | 1.98                     | 0.62              |
| 1:1A:2587:A:H5'    | 1:1A:2588:C:C5     | 2.34                     | 0.62              |
| 8:1H:243:THR:OG1   | 8:1H:246:ARG:HG2   | 1.99                     | 0.62              |
| 13:2E:12:MET:CE    | 13:2E:137:PRO:HB2  | 2.29                     | 0.62              |
| 20:2L:173:ARG:HA   | 20:2L:176:ARG:HE   | 1.62                     | 0.62              |
| 47:2m:521:A:H2'    | 47:2m:522:A:O4'    | 1.99                     | 0.62              |
| 47:2m:589:G:O3'    | 47:2m:590:A:H2'    | 1.99                     | 0.62              |
| 47:2m:1311:C:OP2   | 72:3J:36:ARG:NH2   | 2.32                     | 0.62              |
| 47:2m:1551:U:O2'   | 47:2m:1578:U:O4    | 2.16                     | 0.62              |
| 49:2o:52:THR:HG23  | 49:2o:56:LYS:O     | 1.99                     | 0.62              |
| 52:2r:50:PRO:CG    | 52:2r:90:VAL:HG13  | 2.28                     | 0.62              |
| 52:2r:180:ALA:HA   | 52:2r:190:ILE:CD1  | 2.29                     | 0.62              |
| 54:2t:56:ARG:HA    | 54:2t:180:GLY:HA2  | 1.81                     | 0.62              |
| 55:2u:21:MET:HE1   | 55:2u:23:ALA:HB2   | 1.80                     | 0.62              |
| 58:2x:113:ILE:HD11 | 58:2x:120:LEU:HD12 | 1.80                     | 0.62              |
| 60:2z:41:ALA:O     | 60:2z:44:VAL:HG22  | 1.98                     | 0.62              |
| 72:3J:91:LEU:HD12  | 72:3J:104:VAL:O    | 1.99                     | 0.62              |
| 75:3M:26:LEU:HB2   | 78:3P:7:LEU:HD13   | 1.80                     | 0.62              |
| 77:3O:62:VAL:HG22  | 77:3O:63:PRO:CD    | 2.28                     | 0.62              |
| 77:3O:65:TYR:HA    | 77:3O:111:ARG:HH21 | 1.63                     | 0.62              |
| 1:1A:15:A:O2'      | 1:1A:16:G:H5'      | 1.98                     | 0.62              |
| 1:1A:351:C:H2'     | 1:1A:352:G:O4'     | 1.98                     | 0.62              |
| 1:1A:2060:G:O2'    | 1:1A:2061:U:H5'    | 1.99                     | 0.62              |
| 1:1A:4742:G:H2'    | 1:1A:4743:G:C8     | 2.34                     | 0.62              |
| 1:1A:4772:C:H2'    | 1:1A:4773:C:C4     | 2.34                     | 0.62              |
| 1:1A:4874:A:C2     | 17:2I:175:MET:HG3  | 2.34                     | 0.62              |
| 25:2Q:45:ASN:OD1   | 25:2Q:47:ARG:HB2   | 1.99                     | 0.62              |
| 26:2R:93:ASN:HB2   | 26:2R:95:THR:CG2   | 2.29                     | 0.62              |
| 36:2b:107:GLN:NE2  | 36:2b:111:GLU:OE2  | 2.32                     | 0.62              |
| 47:2m:12:U:H2'     | 47:2m:13:C:H6      | 1.64                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1086:G:O2'   | 47:2m:1087:A:H5'   | 1.98                     | 0.62              |
| 47:2m:1105:G:O3'   | 78:3P:69:GLY:HA3   | 2.00                     | 0.62              |
| 47:2m:1388:A:H61   | 50:2p:161:GLY:HA2  | 1.64                     | 0.62              |
| 47:2m:1418:C:OP1   | 47:2m:1418:C:H3'   | 2.00                     | 0.62              |
| 53:2s:40:LEU:HD23  | 53:2s:40:LEU:O     | 2.00                     | 0.62              |
| 66:3D:12:ALA:C     | 66:3D:55:VAL:HG23  | 2.24                     | 0.62              |
| 71:3I:102:ILE:HD12 | 71:3I:103:GLU:N    | 2.15                     | 0.62              |
| 77:3O:54:THR:CG2   | 77:3O:78:LYS:HD3   | 2.30                     | 0.62              |
| 1:1A:2018:C:O2'    | 1:1A:2019:C:O5'    | 2.15                     | 0.62              |
| 1:1A:2886:U:O2'    | 1:1A:2887:U:H5'    | 1.98                     | 0.62              |
| 1:1A:4526:U:C2'    | 1:1A:4527:G:H5'    | 2.28                     | 0.62              |
| 1:1A:4619:U:H2'    | 1:1A:4620:U:C6     | 2.35                     | 0.62              |
| 4:1D:137:ILE:HD11  | 4:1D:149:LYS:HB2   | 1.81                     | 0.62              |
| 30:2V:40:LEU:O     | 30:2V:44:ARG:HG3   | 2.00                     | 0.62              |
| 37:2c:2:ALA:N      | 37:2c:5:TYR:HH     | 1.97                     | 0.62              |
| 47:2m:147:A:O2'    | 47:2m:148:U:O5'    | 2.18                     | 0.62              |
| 47:2m:1291:A:H3'   | 47:2m:1292:C:H5'   | 1.81                     | 0.62              |
| 52:2r:20:PHE:CE2   | 52:2r:94:LYS:HB2   | 2.35                     | 0.62              |
| 59:2y:24:LEU:CD1   | 59:2y:58:MET:HG2   | 2.29                     | 0.62              |
| 76:3N:7:ILE:HG23   | 76:3N:25:ILE:HG23  | 1.80                     | 0.62              |
| 1:1A:758:G:H5'     | 11:2C:51:LYS:CE    | 2.29                     | 0.62              |
| 1:1A:2026:A:H2'    | 1:1A:2027:U:H6     | 1.65                     | 0.62              |
| 6:1F:76:ILE:HG13   | 6:1F:77:PRO:HD2    | 1.80                     | 0.62              |
| 14:2F:77:SER:OG    | 14:2F:80:GLU:HG3   | 1.99                     | 0.62              |
| 47:2m:636:C:H2'    | 47:2m:637:U:C6     | 2.34                     | 0.62              |
| 47:2m:866:U:H3     | 47:2m:867:G:N2     | 1.97                     | 0.62              |
| 47:2m:1115:U:H4'   | 47:2m:1116:C:OP1   | 1.98                     | 0.62              |
| 47:2m:1519:U:H1'   | 60:2z:135:HIS:CE1  | 2.33                     | 0.62              |
| 47:2m:1584:G:O4'   | 47:2m:1586:U:H4'   | 2.00                     | 0.62              |
| 47:2m:1859:A:O2'   | 47:2m:1860:A:H5'   | 1.99                     | 0.62              |
| 48:2n:52:LYS:NZ    | 63:3A:83:PHE:HA    | 2.14                     | 0.62              |
| 50:2p:64:ARG:NH2   | 55:2u:71:LEU:O     | 2.32                     | 0.62              |
| 50:2p:213:PRO:HD3  | 59:2y:19:LYS:CE    | 2.30                     | 0.62              |
| 51:2q:18:TRP:HH2   | 51:2q:31:PRO:HD3   | 1.63                     | 0.62              |
| 56:2v:129:GLY:HA3  | 56:2v:143:LEU:HD11 | 1.82                     | 0.62              |
| 58:2x:88:ILE:HG13  | 58:2x:89:SER:N     | 2.15                     | 0.62              |
| 74:3L:97:LEU:HD22  | 74:3L:98:ARG:N     | 2.14                     | 0.62              |
| 1:1A:172:C:H4'     | 1:1A:173:C:OP1     | 1.99                     | 0.62              |
| 1:1A:1086:C:O2'    | 1:1A:1087:A:H5'    | 1.99                     | 0.62              |
| 1:1A:4459:U:H2'    | 1:1A:4460:U:H6     | 1.62                     | 0.62              |
| 5:1E:10:ARG:NH2    | 5:1E:265:SER:O     | 2.33                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:2E:64:ARG:O     | 43:2i:103:VAL:HG23 | 1.99                     | 0.62              |
| 16:2H:159:ARG:HB3  | 16:2H:164:LEU:HB2  | 1.82                     | 0.62              |
| 20:2L:84:THR:HG23  | 20:2L:87:ALA:H     | 1.65                     | 0.62              |
| 26:2R:40:ILE:HG22  | 26:2R:42:THR:HG23  | 1.82                     | 0.62              |
| 47:2m:339:A:H4'    | 47:2m:340:C:O5'    | 1.99                     | 0.62              |
| 47:2m:354:U:OP2    | 56:2v:107:LYS:HE2  | 1.99                     | 0.62              |
| 47:2m:616:A:H1'    | 79:3Q:12:VAL:HG23  | 1.80                     | 0.62              |
| 47:2m:1112:U:H2'   | 47:2m:1113:A:C4'   | 2.21                     | 0.62              |
| 47:2m:1313:A:H5'   | 47:2m:1314:U:H5    | 1.65                     | 0.62              |
| 47:2m:1522:A:OP1   | 60:2z:144:ARG:NH1  | 2.32                     | 0.62              |
| 47:2m:1644:C:O2'   | 47:2m:1645:C:H5'   | 1.99                     | 0.62              |
| 48:2n:77:ILE:CD1   | 48:2n:99:ILE:HB    | 2.29                     | 0.62              |
| 69:3G:65:LYS:HG2   | 69:3G:273:LEU:HD13 | 1.81                     | 0.62              |
| 77:3O:98:LYS:CG    | 77:3O:110:THR:HG23 | 2.28                     | 0.62              |
| 1:1A:73:A:OP1      | 14:2F:106:SER:OG   | 2.05                     | 0.62              |
| 1:1A:163:A:H2'     | 1:1A:164:G:H8      | 1.63                     | 0.62              |
| 1:1A:1332:C:H2'    | 1:1A:1333:A:C8     | 2.32                     | 0.62              |
| 1:1A:1749:A:H2'    | 1:1A:1750:G:C8     | 2.35                     | 0.62              |
| 1:1A:2539:C:H2'    | 1:1A:2540:C:H6     | 1.64                     | 0.62              |
| 1:1A:3941:G:O2'    | 1:1A:3942:A:H5'    | 1.99                     | 0.62              |
| 1:1A:4109:G:H2'    | 1:1A:4110:C:C6     | 2.35                     | 0.62              |
| 1:1A:4242:U:H4'    | 1:1A:4243:C:OP1    | 2.00                     | 0.62              |
| 1:1A:5015:G:H2'    | 1:1A:5016:A:C2     | 2.34                     | 0.62              |
| 5:1E:107:ALA:HB2   | 5:1E:201:LEU:CG    | 2.30                     | 0.62              |
| 16:2H:96:ARG:NH2   | 16:2H:104:GLU:OE1  | 2.32                     | 0.62              |
| 47:2m:168:C:H4'    | 47:2m:168:C:OP1    | 1.99                     | 0.62              |
| 47:2m:1237:C:H2'   | 47:2m:1238:U:O4'   | 2.00                     | 0.62              |
| 47:2m:1402:A:H1'   | 62:2i:54:VAL:HG22  | 1.82                     | 0.62              |
| 47:2m:1665:G:OP2   | 61:20:89:PRO:HG2   | 1.99                     | 0.62              |
| 50:2p:33:GLY:HA3   | 50:2p:53:THR:CG2   | 2.30                     | 0.62              |
| 51:2q:128:LYS:O    | 51:2q:129:ILE:HD12 | 1.99                     | 0.62              |
| 53:2s:137:SER:OG   | 53:2s:162:GLN:HB2  | 1.99                     | 0.62              |
| 54:2t:172:LEU:HD12 | 54:2t:190:LEU:HB2  | 1.81                     | 0.62              |
| 68:3F:226:HIS:O    | 68:3F:227:LEU:HD22 | 1.99                     | 0.62              |
| 68:3F:258:ILE:HD12 | 68:3F:268:ASP:CB   | 2.27                     | 0.62              |
| 73:3K:93:LYS:HB2   | 73:3K:150:VAL:CG2  | 2.30                     | 0.62              |
| 1:1A:1405:C:N4     | 1:1A:1408:G:N3     | 2.45                     | 0.62              |
| 1:1A:2415:U:H2'    | 1:1A:2416:G:O4'    | 1.99                     | 0.62              |
| 1:1A:2485:U:O2'    | 1:1A:2486:G:N2     | 2.33                     | 0.62              |
| 1:1A:2704:C:H2'    | 1:1A:2705:G:O4'    | 1.99                     | 0.62              |
| 1:1A:2833:A:OP2    | 32:2X:44:ARG:NH2   | 2.31                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:1C:19:C:H2'     | 3:1C:20:A:C8       | 2.35                     | 0.62              |
| 8:1H:155:GLY:O    | 8:1H:158:ARG:NH1   | 2.33                     | 0.62              |
| 21:2M:71:SER:O    | 21:2M:76:LYS:NZ    | 2.33                     | 0.62              |
| 46:2l:131:ALA:HB3 | 46:2l:133:LYS:CE   | 2.30                     | 0.62              |
| 47:2m:154:U:O2'   | 70:3H:4:ASN:OD1    | 2.16                     | 0.62              |
| 47:2m:1616:U:H2'  | 47:2m:1617:G:C8    | 2.34                     | 0.62              |
| 48:2n:137:ALA:HA  | 48:2n:142:LEU:HD21 | 1.80                     | 0.62              |
| 51:2q:48:LEU:HD13 | 51:2q:64:ILE:HD11  | 1.82                     | 0.62              |
| 52:2r:76:MET:CE   | 52:2r:169:ILE:HD11 | 2.29                     | 0.62              |
| 53:2s:28:LEU:O    | 53:2s:31:GLU:HG2   | 2.00                     | 0.62              |
| 59:2y:60:ARG:HG3  | 59:2y:63:ARG:HH21  | 1.65                     | 0.62              |
| 61:20:101:ARG:O   | 61:20:105:GLN:HG3  | 1.99                     | 0.62              |
| 73:3K:4:MET:HE2   | 73:3K:124:ARG:CZ   | 2.30                     | 0.62              |
| 1:1A:375:G:OP2    | 38:2d:52:LYS:NZ    | 2.22                     | 0.62              |
| 1:1A:491:G:H2'    | 1:1A:492:U:C6      | 2.34                     | 0.62              |
| 1:1A:914:U:O2'    | 1:1A:915:A:OP2     | 2.14                     | 0.62              |
| 1:1A:1196:G:H2'   | 1:1A:1197:C:H6     | 1.65                     | 0.62              |
| 1:1A:1461:C:H2'   | 1:1A:1462:A:H8     | 1.65                     | 0.62              |
| 10:2B:55:VAL:HG12 | 26:2R:44:PRO:HA    | 1.82                     | 0.62              |
| 13:2E:23:ASN:HB3  | 13:2E:129:ASP:OD1  | 2.00                     | 0.62              |
| 23:2O:49:VAL:HG21 | 23:2O:57:GLY:CA    | 2.30                     | 0.62              |
| 34:2Z:104:MET:O   | 34:2Z:105:LEU:HB3  | 2.00                     | 0.62              |
| 47:2m:1256:G:C8   | 67:3E:40:ARG:HD3   | 2.35                     | 0.62              |
| 47:2m:1262:C:H42  | 67:3E:15:GLY:HA3   | 1.64                     | 0.62              |
| 47:2m:1389:C:H4'  | 50:2p:205:PRO:HG3  | 1.80                     | 0.62              |
| 47:2m:1705:C:H2'  | 47:2m:1706:G:C8    | 2.34                     | 0.62              |
| 47:2m:1724:A:O2'  | 47:2m:1725:U:H5'   | 2.00                     | 0.62              |
| 47:2m:1784:G:O2'  | 47:2m:1785:C:H5'   | 2.00                     | 0.62              |
| 50:2p:18:LYS:HA   | 50:2p:21:LEU:CD2   | 2.29                     | 0.62              |
| 58:2x:50:LYS:HA   | 58:2x:53:GLU:CG    | 2.30                     | 0.62              |
| 60:2z:14:ARG:NH1  | 60:2z:14:ARG:HB3   | 2.14                     | 0.62              |
| 60:2z:21:ASP:OD1  | 60:2z:23:ARG:N     | 2.33                     | 0.62              |
| 64:3B:89:GLY:O    | 64:3B:92:ASN:ND2   | 2.32                     | 0.62              |
| 70:3H:30:LYS:O    | 70:3H:102:VAL:HG22 | 2.00                     | 0.62              |
| 74:3L:99:ALA:H    | 74:3L:133:THR:HG23 | 1.63                     | 0.62              |
| 76:3N:88:LYS:HB3  | 76:3N:97:TYR:CD2   | 2.35                     | 0.62              |
| 1:1A:385:A:N3     | 1:1A:387:G:H5''    | 2.14                     | 0.61              |
| 1:1A:499:G:HO2'   | 1:1A:500:G:P       | 2.23                     | 0.61              |
| 1:1A:518:G:H22    | 1:1A:643:C:H2'     | 1.65                     | 0.61              |
| 1:1A:2611:A:H2'   | 1:1A:2612:G:C8     | 2.35                     | 0.61              |
| 1:1A:2638:G:H1    | 1:1A:2697:A:H61    | 1.46                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2696:A:H62    | 39:2e:35:LYS:HE2   | 1.65                     | 0.61              |
| 13:2E:12:MET:HA    | 13:2E:12:MET:CE    | 2.29                     | 0.61              |
| 26:2R:79:PHE:CD1   | 36:2b:36:VAL:HG21  | 2.35                     | 0.61              |
| 47:2m:60:A:N3      | 47:2m:317:C:O2'    | 2.33                     | 0.61              |
| 47:2m:164:A:O2'    | 47:2m:165:G:H5'    | 2.00                     | 0.61              |
| 47:2m:902:G:N1     | 47:2m:903:A:O2'    | 2.30                     | 0.61              |
| 47:2m:1457:U:H2'   | 47:2m:1458:G:C8    | 2.34                     | 0.61              |
| 53:2s:99:ARG:HG3   | 53:2s:99:ARG:O     | 1.99                     | 0.61              |
| 56:2v:127:THR:HB   | 56:2v:144:LYS:HE3  | 1.81                     | 0.61              |
| 57:2w:61:ARG:O     | 57:2w:65:LYS:HG2   | 2.00                     | 0.61              |
| 59:2y:43:SER:OG    | 59:2y:46:LEU:HB3   | 2.00                     | 0.61              |
| 60:2z:12:ILE:HD12  | 60:2z:19:ASN:HB2   | 1.82                     | 0.61              |
| 68:3F:129:ILE:HG21 | 68:3F:177:TRP:CZ3  | 2.34                     | 0.61              |
| 68:3F:291:TRP:CE3  | 68:3F:298:LEU:HG   | 2.35                     | 0.61              |
| 1:1A:187:U:H4'     | 1:1A:189:G:OP2     | 1.99                     | 0.61              |
| 1:1A:1317:U:H2'    | 1:1A:1318:C:C6     | 2.35                     | 0.61              |
| 1:1A:1333:A:H2'    | 1:1A:1334:A:H8     | 1.63                     | 0.61              |
| 1:1A:3861:A:H2'    | 1:1A:3862:A:C8     | 2.35                     | 0.61              |
| 81:1A:5118:84D:N   | 43:2i:86:LYS:HE2   | 2.15                     | 0.61              |
| 23:2O:19:LEU:CB    | 23:2O:74:SER:H     | 2.13                     | 0.61              |
| 46:2l:54:ARG:CG    | 46:2l:152:LYS:HD2  | 2.26                     | 0.61              |
| 47:2m:158:A:H2'    | 47:2m:159:A:H1'    | 1.81                     | 0.61              |
| 47:2m:557:U:H2'    | 47:2m:558:G:O4'    | 2.00                     | 0.61              |
| 47:2m:1392:U:OP1   | 62:21:83:ARG:NH2   | 2.32                     | 0.61              |
| 47:2m:1442:U:H2'   | 47:2m:1443:C:C6    | 2.34                     | 0.61              |
| 47:2m:1558:C:H2'   | 47:2m:1559:C:C6    | 2.35                     | 0.61              |
| 47:2m:1562:C:H4'   | 61:20:120:GLY:H    | 1.65                     | 0.61              |
| 51:2q:167:GLY:O    | 51:2q:168:LYS:HD3  | 2.00                     | 0.61              |
| 52:2r:67:PRO:HD2   | 52:2r:70:GLU:OE1   | 1.99                     | 0.61              |
| 54:2t:129:LEU:HB3  | 54:2t:133:GLU:OE1  | 1.99                     | 0.61              |
| 56:2v:40:ILE:HD12  | 56:2v:143:LEU:HD23 | 1.82                     | 0.61              |
| 64:3B:32:LEU:HD21  | 64:3B:34:THR:CG2   | 2.30                     | 0.61              |
| 68:3F:297:THR:CG2  | 68:3F:311:GLN:HG2  | 2.27                     | 0.61              |
| 69:3G:210:PRO:O    | 69:3G:213:LEU:HD23 | 2.00                     | 0.61              |
| 73:3K:124:ARG:O    | 73:3K:127:ARG:HG2  | 1.99                     | 0.61              |
| 1:1A:939:G:O2'     | 1:1A:940:C:H5'     | 2.01                     | 0.61              |
| 1:1A:1069:G:H2'    | 1:1A:1070:G:O4'    | 1.99                     | 0.61              |
| 1:1A:2907:G:H4'    | 1:1A:3590:G:H1     | 1.65                     | 0.61              |
| 1:1A:4120:U:O2'    | 35:2a:93:ARG:NH1   | 2.32                     | 0.61              |
| 12:2D:36:LEU:HD11  | 12:2D:69:ARG:NH1   | 2.15                     | 0.61              |
| 17:2I:14:HIS:CE1   | 17:2I:119:VAL:HG13 | 2.35                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:2N:57:TYR:OH    | 22:2N:87:LYS:HE3   | 2.00                     | 0.61              |
| 43:2i:56:PHE:CZ    | 43:2i:58:LYS:HB2   | 2.36                     | 0.61              |
| 47:2m:1712:A:H2'   | 47:2m:1713:C:H6    | 1.65                     | 0.61              |
| 49:2o:146:ARG:HB2  | 49:2o:149:GLN:HB2  | 1.82                     | 0.61              |
| 49:2o:185:VAL:HA   | 49:2o:188:LEU:HG   | 1.81                     | 0.61              |
| 52:2r:32:ASP:OD2   | 52:2r:35:LEU:N     | 2.25                     | 0.61              |
| 59:2y:46:LEU:HD11  | 59:2y:50:ILE:HD11  | 1.83                     | 0.61              |
| 63:3A:1:MET:HE2    | 69:3G:254:ASP:HB2  | 1.81                     | 0.61              |
| 68:3F:70:VAL:HG23  | 68:3F:113:PHE:CD2  | 2.35                     | 0.61              |
| 68:3F:79:LEU:CD1   | 68:3F:120:ILE:HG12 | 2.31                     | 0.61              |
| 68:3F:119:GLN:OE1  | 68:3F:119:GLN:N    | 2.33                     | 0.61              |
| 70:3H:58:LYS:HA    | 70:3H:107:SER:OG   | 2.01                     | 0.61              |
| 1:1A:983:C:H2'     | 1:1A:984:C:C6      | 2.36                     | 0.61              |
| 1:1A:992:C:C2'     | 1:1A:993:G:H5'     | 2.30                     | 0.61              |
| 1:1A:1970:A:O2'    | 1:1A:2018:C:N4     | 2.33                     | 0.61              |
| 1:1A:2669:C:O2'    | 1:1A:2670:C:O4'    | 2.13                     | 0.61              |
| 1:1A:4513:A:OP2    | 81:1A:5109:84D:N2  | 2.33                     | 0.61              |
| 1:1A:5006:U:H4'    | 1:1A:5007:A:H5'    | 1.83                     | 0.61              |
| 11:2C:88:PHE:CE1   | 11:2C:151:ILE:HD12 | 2.36                     | 0.61              |
| 12:2D:152:LEU:HB3  | 12:2D:165:ILE:HD12 | 1.83                     | 0.61              |
| 16:2H:115:VAL:HG22 | 16:2H:134:LEU:HD11 | 1.81                     | 0.61              |
| 21:2M:7:LEU:O      | 21:2M:103:ALA:HB1  | 2.01                     | 0.61              |
| 35:2a:60:ARG:HB2   | 35:2a:63:VAL:CG1   | 2.30                     | 0.61              |
| 39:2e:23:VAL:HG22  | 39:2e:36:VAL:HG22  | 1.81                     | 0.61              |
| 47:2m:17:C:H2'     | 47:2m:18:C:C6      | 2.36                     | 0.61              |
| 47:2m:308:G:O2'    | 54:2t:45:THR:HG21  | 2.01                     | 0.61              |
| 47:2m:641:A:OP1    | 71:3I:40:LYS:HD2   | 2.00                     | 0.61              |
| 47:2m:690:G:H2'    | 47:2m:691:G:H5''   | 1.81                     | 0.61              |
| 47:2m:996:A:H2'    | 47:2m:997:A:C8     | 2.34                     | 0.61              |
| 47:2m:1259:A:H3'   | 47:2m:1259:A:N3    | 2.16                     | 0.61              |
| 50:2p:55:THR:CA    | 50:2p:58:VAL:HG12  | 2.28                     | 0.61              |
| 52:2r:70:GLU:O     | 52:2r:73:THR:HG22  | 2.01                     | 0.61              |
| 68:3F:121:VAL:HG23 | 68:3F:131:LEU:HD21 | 1.83                     | 0.61              |
| 76:3N:20:ARG:HD3   | 76:3N:76:TYR:CE1   | 2.35                     | 0.61              |
| 77:3O:97:ILE:CD1   | 77:3O:111:ARG:HA   | 2.31                     | 0.61              |
| 1:1A:2389:A:H5'    | 32:2X:70:LYS:HD2   | 1.81                     | 0.61              |
| 1:1A:4174:U:H2'    | 1:1A:4175:G:H8     | 1.66                     | 0.61              |
| 1:1A:4717:A:C2'    | 1:1A:4718:G:H5'    | 2.31                     | 0.61              |
| 25:2Q:52:THR:HG22  | 25:2Q:54:LEU:H     | 1.66                     | 0.61              |
| 47:2m:126:G:H4'    | 47:2m:215:G:H21    | 1.65                     | 0.61              |
| 47:2m:148:U:O2'    | 47:2m:149:A:O5'    | 2.15                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:349:A:H2'    | 47:2m:350:C:C6     | 2.35                     | 0.61              |
| 47:2m:1137:U:O2'   | 48:2n:155:ARG:NH2  | 2.33                     | 0.61              |
| 47:2m:1153:C:OP2   | 75:3M:71:LYS:NZ    | 2.26                     | 0.61              |
| 47:2m:1413:G:OP2   | 47:2m:1413:G:H3'   | 2.01                     | 0.61              |
| 47:2m:1604:G:C2'   | 47:2m:1605:G:H5'   | 2.31                     | 0.61              |
| 47:2m:1671:G:H2'   | 47:2m:1672:U:C6    | 2.35                     | 0.61              |
| 47:2m:1782:G:H2'   | 47:2m:1783:C:H4'   | 1.81                     | 0.61              |
| 52:2r:51:HIS:CD2   | 52:2r:86:LYS:HG2   | 2.36                     | 0.61              |
| 52:2r:88:MET:O     | 52:2r:91:ARG:HG2   | 2.00                     | 0.61              |
| 52:2r:175:ASP:HA   | 52:2r:178:ILE:CD1  | 2.29                     | 0.61              |
| 54:2t:143:LYS:O    | 54:2t:147:LYS:HG2  | 2.00                     | 0.61              |
| 58:2x:49:TYR:HA    | 58:2x:52:LEU:HD11  | 1.81                     | 0.61              |
| 67:3E:19:ARG:NE    | 67:3E:32:ARG:HD3   | 2.15                     | 0.61              |
| 68:3F:212:LYS:HA   | 68:3F:235:ILE:HG13 | 1.83                     | 0.61              |
| 68:3F:289:LEU:HD13 | 68:3F:290:ALA:N    | 2.15                     | 0.61              |
| 1:1A:128:C:H2'     | 1:1A:129:C:O4'     | 2.01                     | 0.61              |
| 1:1A:2063:G:O2'    | 1:1A:2064:G:H5'    | 2.01                     | 0.61              |
| 1:1A:4868:G:C2'    | 1:1A:4869:U:H5''   | 2.30                     | 0.61              |
| 9:2A:144:TYR:CE2   | 9:2A:237:GLU:HG3   | 2.35                     | 0.61              |
| 12:2D:30:LYS:HG3   | 12:2D:63:GLU:HG3   | 1.82                     | 0.61              |
| 47:2m:291:G:O2'    | 47:2m:292:A:H5''   | 2.00                     | 0.61              |
| 47:2m:892:U:O2'    | 47:2m:893:U:OP1    | 2.17                     | 0.61              |
| 47:2m:1009:A:O2'   | 47:2m:1010:G:H5'   | 1.99                     | 0.61              |
| 49:2o:181:LEU:O    | 49:2o:185:VAL:HG12 | 1.99                     | 0.61              |
| 55:2u:57:TYR:O     | 55:2u:72:THR:OG1   | 2.17                     | 0.61              |
| 58:2x:54:PRO:CG    | 58:2x:88:ILE:HD11  | 2.30                     | 0.61              |
| 60:2z:114:LEU:O    | 60:2z:117:ILE:HG22 | 2.01                     | 0.61              |
| 70:3H:200:LYS:HG2  | 70:3H:204:GLU:OE2  | 1.99                     | 0.61              |
| 76:3N:6:THR:C      | 76:3N:7:ILE:HD13   | 2.26                     | 0.61              |
| 77:3O:100:VAL:HB   | 77:3O:108:ILE:CG2  | 2.30                     | 0.61              |
| 1:1A:253:G:O2'     | 1:1A:254:G:H5'     | 2.01                     | 0.61              |
| 1:1A:690:C:OP1     | 45:2k:87:ARG:NH1   | 2.32                     | 0.61              |
| 1:1A:1262:G:H2'    | 1:1A:1263:A:C8     | 2.36                     | 0.61              |
| 1:1A:2003:G:H1     | 1:1A:2016:C:H42    | 1.48                     | 0.61              |
| 1:1A:2465:C:C1'    | 1:1A:3672:G:H22    | 2.08                     | 0.61              |
| 1:1A:2762:G:O2'    | 1:1A:2763:U:OP2    | 2.14                     | 0.61              |
| 1:1A:4081:G:O2'    | 1:1A:4082:G:H5'    | 2.00                     | 0.61              |
| 5:1E:160:ILE:HD12  | 5:1E:193:LYS:HG3   | 1.82                     | 0.61              |
| 9:2A:52:GLU:HG3    | 30:2V:96:LEU:HD13  | 1.83                     | 0.61              |
| 47:2m:464:A:H3'    | 47:2m:465:A:H8     | 1.65                     | 0.61              |
| 47:2m:509:G:OP1    | 71:3I:2:PRO:HA     | 2.01                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:525:A:H2'   | 47:2m:526:A:C8     | 2.32                     | 0.61              |
| 47:2m:738:C:H3'   | 47:2m:738:C:O2     | 2.00                     | 0.61              |
| 47:2m:1599:U:C5   | 52:2r:166:ILE:HD12 | 2.36                     | 0.61              |
| 47:2m:1862:G:H4'  | 47:2m:1863:A:OP1   | 2.00                     | 0.61              |
| 52:2r:171:GLU:OE2 | 77:3O:106:GLN:HG3  | 2.00                     | 0.61              |
| 62:21:81:GLN:OE1  | 67:3E:55:LEU:HB2   | 2.00                     | 0.61              |
| 68:3F:5:MET:SD    | 68:3F:270:LEU:HD11 | 2.40                     | 0.61              |
| 68:3F:217:MET:HB3 | 68:3F:229:THR:CG2  | 2.30                     | 0.61              |
| 70:3H:28:TYR:HB3  | 70:3H:29:GLU:OE1   | 2.00                     | 0.61              |
| 70:3H:49:VAL:CG2  | 70:3H:115:LYS:HE3  | 2.30                     | 0.61              |
| 72:3J:51:VAL:HG13 | 72:3J:109:VAL:HG23 | 1.83                     | 0.61              |
| 1:1A:272:U:H2'    | 1:1A:273:U:C6      | 2.35                     | 0.61              |
| 1:1A:674:G:H2'    | 1:1A:675:C:C6      | 2.36                     | 0.61              |
| 1:1A:1759:G:O6    | 1:1A:1760:G:N2     | 2.34                     | 0.61              |
| 1:1A:2544:G:OP2   | 1:1A:2546:G:N2     | 2.31                     | 0.61              |
| 1:1A:2706:G:H3'   | 1:1A:2707:U:H5'    | 1.83                     | 0.61              |
| 1:1A:4600:G:H4'   | 1:1A:4601:U:O5'    | 2.00                     | 0.61              |
| 1:1A:5026:U:H1'   | 1:1A:5027:C:C5     | 2.36                     | 0.61              |
| 2:1B:111:C:H2'    | 2:1B:112:U:O4'     | 1.99                     | 0.61              |
| 3:1C:141:C:H2'    | 3:1C:142:U:C6      | 2.34                     | 0.61              |
| 20:2L:144:LYS:HD3 | 20:2L:144:LYS:N    | 2.16                     | 0.61              |
| 47:2m:921:G:C5    | 75:3M:28:ARG:HD2   | 2.36                     | 0.61              |
| 47:2m:1286:G:N2   | 72:3J:33:ARG:HG3   | 2.16                     | 0.61              |
| 47:2m:1497:G:H4'  | 47:2m:1498:A:O5'   | 2.00                     | 0.61              |
| 47:2m:1516:G:O2'  | 47:2m:1517:G:O5'   | 2.19                     | 0.61              |
| 47:2m:1617:G:N2   | 47:2m:1619:A:H3'   | 2.16                     | 0.61              |
| 50:2p:106:ARG:CG  | 50:2p:175:VAL:HG22 | 2.31                     | 0.61              |
| 61:20:133:ARG:HD3 | 61:20:134:ILE:HG23 | 1.80                     | 0.61              |
| 68:3F:177:TRP:HD1 | 68:3F:184:LEU:HA   | 1.64                     | 0.61              |
| 68:3F:232:GLY:HA3 | 68:3F:259:TRP:CH2  | 2.36                     | 0.61              |
| 76:3N:111:LYS:HG3 | 76:3N:114:MET:HE3  | 1.82                     | 0.61              |
| 1:1A:705:G:H2'    | 1:1A:706:C:H6      | 1.64                     | 0.61              |
| 1:1A:746:A:O2'    | 1:1A:747:A:H5'     | 2.01                     | 0.61              |
| 1:1A:2485:U:OP1   | 1:1A:2486:G:H5'    | 2.01                     | 0.61              |
| 1:1A:3950:U:H5''  | 1:1A:3951:G:N7     | 2.15                     | 0.61              |
| 1:1A:4042:G:OP1   | 46:2l:101:LYS:NZ   | 2.31                     | 0.61              |
| 1:1A:4738:C:O2'   | 1:1A:4739:C:H5'    | 2.01                     | 0.61              |
| 1:1A:4868:G:H2'   | 1:1A:4869:U:H5''   | 1.82                     | 0.61              |
| 1:1A:4885:U:H5    | 8:1H:272:ARG:HH22  | 1.47                     | 0.61              |
| 3:1C:86:U:H3'     | 36:2b:5:LYS:NZ     | 2.16                     | 0.61              |
| 6:1F:268:ARG:HG2  | 6:1F:268:ARG:HH11  | 1.66                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:2A:226:HIS:ND1   | 9:2A:228:VAL:HG22  | 2.15                     | 0.61              |
| 10:2B:88:ASP:HB3   | 10:2B:91:THR:HG22  | 1.82                     | 0.61              |
| 10:2B:220:GLU:O    | 10:2B:224:THR:HG23 | 2.01                     | 0.61              |
| 12:2D:179:ASP:OD1  | 12:2D:180:GLU:N    | 2.34                     | 0.61              |
| 13:2E:4:ASP:O      | 13:2E:8:LYS:HG2    | 2.01                     | 0.61              |
| 15:2G:123:ILE:HD13 | 17:2I:182:GLU:HG2  | 1.82                     | 0.61              |
| 22:2N:102:ARG:HD3  | 22:2N:106:LEU:HG   | 1.83                     | 0.61              |
| 28:2T:115:LYS:HE3  | 28:2T:119:GLU:OE2  | 2.01                     | 0.61              |
| 47:2m:538:U:H4'    | 47:2m:546:G:C5     | 2.36                     | 0.61              |
| 47:2m:1617:G:H4'   | 67:3E:14:PHE:CE2   | 2.35                     | 0.61              |
| 47:2m:1798:C:H2'   | 47:2m:1799:G:O4'   | 2.00                     | 0.61              |
| 48:2n:12:GLU:HB3   | 59:2y:111:PHE:CE2  | 2.36                     | 0.61              |
| 53:2s:98:ARG:HB3   | 53:2s:125:VAL:CG2  | 2.27                     | 0.61              |
| 59:2y:26:ASN:OD1   | 59:2y:26:ASN:N     | 2.33                     | 0.61              |
| 68:3F:96:THR:HG22  | 68:3F:97:THR:H     | 1.66                     | 0.61              |
| 69:3G:74:LYS:HE3   | 69:3G:269:PHE:CG   | 2.36                     | 0.61              |
| 70:3H:162:LEU:HD11 | 70:3H:170:ARG:HB3  | 1.83                     | 0.61              |
| 1:1A:257:C:H2'     | 1:1A:258:G:C8      | 2.36                     | 0.61              |
| 1:1A:500:G:H4'     | 1:1A:504:G:O5'     | 2.01                     | 0.61              |
| 1:1A:1707:C:C6     | 30:2V:103:LYS:HE2  | 2.36                     | 0.61              |
| 1:1A:2528:G:H21    | 1:1A:2529:A:H5''   | 1.66                     | 0.61              |
| 1:1A:2846:G:O2'    | 24:2P:19:GLY:O     | 2.18                     | 0.61              |
| 1:1A:4869:U:H2'    | 1:1A:4870:G:H5'    | 1.83                     | 0.61              |
| 1:1A:5041:G:OP2    | 25:2Q:61:LYS:HD2   | 1.99                     | 0.61              |
| 6:1F:163:LYS:O     | 6:1F:166:GLU:HG2   | 2.01                     | 0.61              |
| 25:2Q:78:PHE:CG    | 70:3H:9:ALA:HA     | 2.35                     | 0.61              |
| 47:2m:902:G:H2'    | 47:2m:902:G:N3     | 2.16                     | 0.61              |
| 47:2m:919:A:OP2    | 73:3K:64:ARG:NH1   | 2.34                     | 0.61              |
| 47:2m:1259:A:N6    | 47:2m:1518:C:H3'   | 2.16                     | 0.61              |
| 47:2m:1483:A:O2'   | 50:2p:160:SER:HB3  | 2.01                     | 0.61              |
| 47:2m:1648:G:C5'   | 58:2x:125:ARG:HB3  | 2.30                     | 0.61              |
| 49:2o:127:VAL:HB   | 49:2o:176:VAL:HG11 | 1.81                     | 0.61              |
| 50:2p:126:ILE:HG21 | 50:2p:134:CYS:CB   | 2.31                     | 0.61              |
| 51:2q:100:ARG:HH22 | 51:2q:122:LYS:HA   | 1.66                     | 0.61              |
| 52:2r:94:LYS:O     | 52:2r:98:GLU:HG2   | 2.01                     | 0.61              |
| 58:2x:97:GLN:HG2   | 68:3F:60:ARG:HH12  | 1.66                     | 0.61              |
| 61:20:115:LYS:HG2  | 61:20:121:ARG:HG2  | 1.83                     | 0.61              |
| 76:3N:13:MET:O     | 76:3N:13:MET:HG3   | 2.00                     | 0.61              |
| 1:1A:1418:C:C2'    | 1:1A:1419:G:H5'    | 2.31                     | 0.60              |
| 1:1A:1481:C:N4     | 37:2c:4:ARG:HG3    | 2.15                     | 0.60              |
| 6:1F:208:CYS:SG    | 6:1F:230:LEU:HD22  | 2.41                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:2D:101:LYS:HZ3  | 12:2D:112:GLN:HG2  | 1.66                     | 0.60              |
| 27:2S:44:VAL:HG21  | 27:2S:119:LEU:HD23 | 1.83                     | 0.60              |
| 27:2S:82:ILE:HG22  | 27:2S:83:GLU:N     | 2.16                     | 0.60              |
| 29:2U:2:PRO:HG2    | 29:2U:5:LEU:HD12   | 1.82                     | 0.60              |
| 44:2j:8:VAL:O      | 44:2j:11:VAL:HG22  | 2.01                     | 0.60              |
| 47:2m:1237:C:O2'   | 57:2w:129:GLY:HA3  | 2.00                     | 0.60              |
| 47:2m:1360:U:H2'   | 47:2m:1361:G:O4'   | 2.01                     | 0.60              |
| 47:2m:1403:C:H42   | 47:2m:1436:C:H5''  | 1.66                     | 0.60              |
| 47:2m:1444:U:O2'   | 47:2m:1445:U:H5'   | 2.01                     | 0.60              |
| 47:2m:1610:G:OP1   | 60:2z:121:ARG:HD2  | 2.01                     | 0.60              |
| 47:2m:1860:A:H5''  | 65:3C:8:ASN:ND2    | 2.16                     | 0.60              |
| 48:2n:12:GLU:HA    | 48:2n:15:VAL:HG23  | 1.82                     | 0.60              |
| 49:2o:35:ALA:HA    | 49:2o:98:THR:CG2   | 2.31                     | 0.60              |
| 49:2o:144:LYS:CD   | 49:2o:208:HIS:HB3  | 2.31                     | 0.60              |
| 50:2p:12:VAL:HG21  | 67:3E:34:TYR:O     | 2.01                     | 0.60              |
| 50:2p:193:ASP:HB3  | 50:2p:199:GLY:HA3  | 1.82                     | 0.60              |
| 59:2y:12:ALA:O     | 59:2y:15:VAL:HG12  | 2.00                     | 0.60              |
| 71:3I:32:ILE:HD11  | 71:3I:40:LYS:HA    | 1.82                     | 0.60              |
| 71:3I:104:ASP:O    | 71:3I:108:ARG:HG2  | 2.01                     | 0.60              |
| 71:3I:113:GLN:OE1  | 71:3I:113:GLN:HA   | 2.00                     | 0.60              |
| 74:3L:101:GLY:HA3  | 74:3L:134:PRO:HD2  | 1.83                     | 0.60              |
| 1:1A:62:A:N3       | 1:1A:77:U:O2'      | 2.29                     | 0.60              |
| 1:1A:1473:U:O2'    | 1:1A:1474:C:H5'    | 2.01                     | 0.60              |
| 1:1A:4457:U:O2     | 5:1E:252:ALA:HB3   | 2.01                     | 0.60              |
| 5:1E:305:THR:HG21  | 5:1E:366:LYS:O     | 2.00                     | 0.60              |
| 7:1G:164:LYS:HA    | 7:1G:167:VAL:HG22  | 1.83                     | 0.60              |
| 8:1H:180:VAL:HG21  | 8:1H:258:LEU:HD11  | 1.83                     | 0.60              |
| 13:2E:57:VAL:HG21  | 13:2E:60:PHE:CE1   | 2.36                     | 0.60              |
| 39:2e:12:LEU:HD22  | 39:2e:12:LEU:H     | 1.64                     | 0.60              |
| 47:2m:1318:G:O2'   | 47:2m:1319:U:H5'   | 2.00                     | 0.60              |
| 50:2p:124:ARG:O    | 50:2p:128:GLU:HG3  | 2.01                     | 0.60              |
| 59:2y:53:TYR:CZ    | 59:2y:57:LEU:HD21  | 2.36                     | 0.60              |
| 70:3H:121:ILE:HG22 | 70:3H:124:LEU:HB3  | 1.84                     | 0.60              |
| 72:3J:68:LEU:O     | 72:3J:72:HIS:ND1   | 2.30                     | 0.60              |
| 74:3L:110:PRO:O    | 74:3L:113:GLN:NE2  | 2.31                     | 0.60              |
| 77:3O:47:LEU:CD2   | 77:3O:79:ILE:HD12  | 2.28                     | 0.60              |
| 1:1A:423:G:H2'     | 1:1A:424:U:C6      | 2.36                     | 0.60              |
| 1:1A:1813:U:O2'    | 1:1A:1814:C:H5'    | 2.01                     | 0.60              |
| 1:1A:2020:U:C3'    | 1:1A:2021:G:H5''   | 2.31                     | 0.60              |
| 1:1A:4063:U:H3'    | 1:1A:4064:C:C6     | 2.36                     | 0.60              |
| 1:1A:4192:A:O2'    | 1:1A:4193:C:H5'    | 2.01                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4322:G:N2     | 1:1A:4325:A:OP2    | 2.30                     | 0.60              |
| 1:1A:4869:U:O2'    | 1:1A:4870:G:H5'    | 2.01                     | 0.60              |
| 1:1A:4910:G:H4'    | 5:1E:95:THR:HG22   | 1.83                     | 0.60              |
| 5:1E:29:VAL:HG12   | 5:1E:31:SER:H      | 1.67                     | 0.60              |
| 12:2D:101:LYS:O    | 12:2D:103:LEU:HD22 | 2.01                     | 0.60              |
| 21:2M:164:LYS:HE2  | 21:2M:164:LYS:CA   | 2.31                     | 0.60              |
| 25:2Q:101:ARG:O    | 25:2Q:105:ARG:HG2  | 2.00                     | 0.60              |
| 35:2a:107:LEU:HD12 | 35:2a:110:GLN:NE2  | 2.13                     | 0.60              |
| 46:2l:85:MET:HE1   | 46:2l:90:LEU:N     | 2.17                     | 0.60              |
| 47:2m:150:A:N6     | 47:2m:168:C:N4     | 2.36                     | 0.60              |
| 47:2m:309:G:H2'    | 47:2m:310:C:C1'    | 2.31                     | 0.60              |
| 47:2m:536:A:H5''   | 47:2m:537:C:C1'    | 2.31                     | 0.60              |
| 47:2m:944:A:C1'    | 74:3L:136:PRO:HB3  | 2.27                     | 0.60              |
| 47:2m:1568:C:O2'   | 47:2m:1569:A:H5''  | 2.01                     | 0.60              |
| 48:2n:155:ARG:O    | 63:3A:63:GLY:HA2   | 2.01                     | 0.60              |
| 49:2o:100:PHE:CD2  | 49:2o:181:LEU:HD11 | 2.37                     | 0.60              |
| 57:2w:35:GLN:O     | 60:2z:88:LYS:NZ    | 2.33                     | 0.60              |
| 63:3A:23:ILE:CD1   | 69:3G:251:LEU:HB2  | 2.31                     | 0.60              |
| 70:3H:152:ASP:CG   | 70:3H:155:GLN:HB2  | 2.27                     | 0.60              |
| 72:3J:67:ALA:CB    | 80:3R:108:VAL:HG23 | 2.31                     | 0.60              |
| 72:3J:79:VAL:CG2   | 72:3J:85:LEU:HD22  | 2.25                     | 0.60              |
| 77:3O:56:ASP:HA    | 77:3O:59:CYS:SG    | 2.41                     | 0.60              |
| 1:1A:1590:C:H4'    | 1:1A:1591:U:OP2    | 2.00                     | 0.60              |
| 1:1A:1730:U:H4'    | 22:2N:100:LYS:HB2  | 1.82                     | 0.60              |
| 1:1A:4238:G:H2'    | 1:1A:4239:A:H8     | 1.65                     | 0.60              |
| 1:1A:4492:U:O2'    | 1:1A:4512:U:O2     | 2.13                     | 0.60              |
| 1:1A:4751:G:O3'    | 17:2I:4:VAL:HG21   | 2.02                     | 0.60              |
| 5:1E:163:ILE:HG22  | 5:1E:180:LEU:HD22  | 1.82                     | 0.60              |
| 9:2A:80:ASN:HB3    | 22:2N:141:VAL:O    | 2.00                     | 0.60              |
| 28:2T:89:ILE:HD11  | 28:2T:91:LEU:HD22  | 1.83                     | 0.60              |
| 47:2m:31:U:H5'     | 47:2m:596:U:OP1    | 2.01                     | 0.60              |
| 47:2m:57:U:OP1     | 47:2m:504:G:O2'    | 2.20                     | 0.60              |
| 47:2m:81:U:H2'     | 47:2m:82:G:H5'     | 1.82                     | 0.60              |
| 47:2m:590:A:H4'    | 47:2m:591:U:OP2    | 1.99                     | 0.60              |
| 47:2m:615:C:O2     | 79:3Q:11:LYS:HE2   | 2.01                     | 0.60              |
| 47:2m:635:G:O2'    | 47:2m:636:C:H5'    | 2.01                     | 0.60              |
| 47:2m:788:G:H2'    | 47:2m:789:G:N7     | 2.16                     | 0.60              |
| 47:2m:828:G:O2'    | 47:2m:829:C:H5'    | 2.01                     | 0.60              |
| 47:2m:1348:G:H2'   | 47:2m:1349:G:H8    | 1.66                     | 0.60              |
| 48:2n:140:VAL:HG23 | 48:2n:142:LEU:HD22 | 1.83                     | 0.60              |
| 49:2o:58:ALA:O     | 49:2o:62:LEU:HG    | 2.02                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:2o:65:ARG:NH2   | 74:3L:51:GLU:OE2   | 2.17                     | 0.60              |
| 50:2p:13:ALA:O     | 50:2p:16:ILE:HG12  | 2.01                     | 0.60              |
| 51:2q:47:PHE:O     | 51:2q:51:ARG:HB2   | 2.01                     | 0.60              |
| 51:2q:95:THR:CB    | 76:3N:16:ARG:HD3   | 2.23                     | 0.60              |
| 60:2z:54:LYS:HE3   | 60:2z:58:GLU:HB2   | 1.83                     | 0.60              |
| 60:2z:85:ASN:OD1   | 60:2z:86:ARG:HG2   | 2.01                     | 0.60              |
| 61:20:27:LYS:HB3   | 61:20:110:LEU:HD21 | 1.81                     | 0.60              |
| 64:3B:107:ARG:CG   | 64:3B:112:VAL:HG22 | 2.31                     | 0.60              |
| 64:3B:128:VAL:HG13 | 64:3B:133:LEU:HD11 | 1.82                     | 0.60              |
| 68:3F:139:LYS:HG2  | 68:3F:140:TYR:N    | 2.16                     | 0.60              |
| 75:3M:3:ARG:HH12   | 75:3M:28:ARG:NH2   | 1.99                     | 0.60              |
| 1:1A:132:G:H2'     | 1:1A:134:G:OP1     | 2.02                     | 0.60              |
| 1:1A:3782:C:P      | 42:2h:23:ARG:HH22  | 2.25                     | 0.60              |
| 1:1A:3947:A:C2'    | 1:1A:3948:C:H5''   | 2.24                     | 0.60              |
| 7:1G:93:THR:HG23   | 7:1G:93:THR:O      | 2.02                     | 0.60              |
| 10:2B:246:SER:O    | 10:2B:250:ILE:HG13 | 2.01                     | 0.60              |
| 11:2C:12:ILE:CD1   | 11:2C:18:ILE:HD11  | 2.31                     | 0.60              |
| 13:2E:78:LYS:HD3   | 13:2E:81:GLU:OE2   | 2.02                     | 0.60              |
| 14:2F:63:THR:HG22  | 14:2F:65:ARG:N     | 2.17                     | 0.60              |
| 14:2F:87:HIS:HE1   | 14:2F:89:LYS:HG3   | 1.65                     | 0.60              |
| 21:2M:164:LYS:HE2  | 21:2M:164:LYS:HA   | 1.84                     | 0.60              |
| 33:2Y:6:PRO:HG3    | 33:2Y:73:GLY:HA3   | 1.84                     | 0.60              |
| 46:2l:172:VAL:HG11 | 46:2l:179:LEU:HD11 | 1.84                     | 0.60              |
| 47:2m:455:A:H2'    | 47:2m:456:C:H6     | 1.66                     | 0.60              |
| 47:2m:1629:C:H2'   | 47:2m:1630:A:C8    | 2.37                     | 0.60              |
| 47:2m:1854:U:H2'   | 47:2m:1855:G:H8    | 1.67                     | 0.60              |
| 48:2n:69:GLU:CD    | 69:3G:270:THR:HG21 | 2.26                     | 0.60              |
| 50:2p:125:PHE:O    | 50:2p:129:SER:OG   | 2.19                     | 0.60              |
| 59:2y:24:LEU:CD1   | 59:2y:58:MET:HE2   | 2.26                     | 0.60              |
| 60:2z:48:ALA:HB3   | 60:2z:50:ILE:HD11  | 1.83                     | 0.60              |
| 75:3M:11:LEU:HB3   | 75:3M:72:CYS:O     | 2.01                     | 0.60              |
| 1:1A:185:C:H4'     | 1:1A:185:C:OP1     | 2.01                     | 0.60              |
| 1:1A:705:G:H2'     | 1:1A:706:C:C6      | 2.36                     | 0.60              |
| 1:1A:2253:A:C2     | 9:2A:26:ALA:HB3    | 2.34                     | 0.60              |
| 1:1A:3971:G:H2'    | 1:1A:3972:A:H5''   | 1.83                     | 0.60              |
| 35:2a:61:PRO:O     | 35:2a:64:LEU:HB2   | 2.01                     | 0.60              |
| 37:2c:16:LYS:HE2   | 37:2c:16:LYS:HA    | 1.84                     | 0.60              |
| 47:2m:842:C:O2'    | 47:2m:843:C:H5'    | 2.01                     | 0.60              |
| 47:2m:1271:C:H2'   | 67:3E:2:GLY:CA     | 2.31                     | 0.60              |
| 47:2m:1380:C:H2'   | 47:2m:1381:G:O4'   | 2.01                     | 0.60              |
| 51:2q:122:LYS:HG2  | 51:2q:162:ILE:CD1  | 2.31                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:2s:154:ILE:CG2  | 53:2s:185:VAL:HG12 | 2.32                     | 0.60              |
| 60:2z:61:GLU:O     | 60:2z:64:VAL:HG12  | 2.01                     | 0.60              |
| 60:2z:71:MET:SD    | 60:2z:99:LEU:HD13  | 2.40                     | 0.60              |
| 60:2z:125:HIS:CD2  | 60:2z:131:VAL:HG11 | 2.35                     | 0.60              |
| 76:3N:97:TYR:CZ    | 76:3N:99:LYS:HD3   | 2.36                     | 0.60              |
| 76:3N:111:LYS:HG3  | 76:3N:114:MET:CE   | 2.30                     | 0.60              |
| 1:1A:1613:A:H5''   | 4:1D:183:GLY:CA    | 2.31                     | 0.60              |
| 1:1A:1662:C:H2'    | 1:1A:1663:C:C6     | 2.37                     | 0.60              |
| 1:1A:2286:G:O2'    | 1:1A:2287:G:H5'    | 2.01                     | 0.60              |
| 1:1A:2645:G:O2'    | 1:1A:2646:C:H5'    | 2.01                     | 0.60              |
| 1:1A:2848:G:O2'    | 1:1A:3838:U:O4     | 2.14                     | 0.60              |
| 1:1A:3760:A:H3'    | 1:1A:3761:C:C5'    | 2.31                     | 0.60              |
| 1:1A:4096:C:H2'    | 1:1A:4097:G:C8     | 2.37                     | 0.60              |
| 1:1A:4305:G:H22    | 22:2N:87:LYS:CD    | 2.14                     | 0.60              |
| 1:1A:4524:G:OP2    | 1:1A:4524:G:H4'    | 2.01                     | 0.60              |
| 6:1F:254:GLU:O     | 6:1F:258:ARG:HG3   | 2.01                     | 0.60              |
| 47:2m:921:G:C6     | 78:3P:22:LYS:HA    | 2.36                     | 0.60              |
| 47:2m:1399:C:H5'   | 68:3F:100:ARG:CZ   | 2.32                     | 0.60              |
| 47:2m:1601:A:H5''  | 47:2m:1602:U:OP1   | 2.02                     | 0.60              |
| 54:2t:148:LYS:O    | 54:2t:151:GLU:HG3  | 2.01                     | 0.60              |
| 57:2w:17:TYR:CG    | 57:2w:112:ILE:HD11 | 2.37                     | 0.60              |
| 57:2w:75:VAL:HG22  | 57:2w:93:MET:CG    | 2.32                     | 0.60              |
| 58:2x:133:GLY:O    | 58:2x:140:ARG:HD2  | 2.01                     | 0.60              |
| 68:3F:24:THR:OG1   | 68:3F:30:MET:HE1   | 2.01                     | 0.60              |
| 68:3F:26:GLN:HG3   | 68:3F:27:PHE:CD2   | 2.36                     | 0.60              |
| 68:3F:135:LEU:HG   | 68:3F:137:VAL:HG13 | 1.84                     | 0.60              |
| 69:3G:88:ILE:HG21  | 69:3G:94:ILE:HD11  | 1.83                     | 0.60              |
| 73:3K:38:TYR:CE2   | 73:3K:78:LYS:HD2   | 2.36                     | 0.60              |
| 74:3L:143:LYS:HG2  | 74:3L:143:LYS:O    | 2.01                     | 0.60              |
| 77:3O:98:LYS:HG2   | 77:3O:110:THR:CG2  | 2.32                     | 0.60              |
| 1:1A:1220:G:HO2'   | 1:1A:1221:G:P      | 2.25                     | 0.60              |
| 1:1A:2686:G:H5'    | 1:1A:2687:U:OP1    | 2.02                     | 0.60              |
| 1:1A:3656:A:H2'    | 1:1A:3657:U:H6     | 1.67                     | 0.60              |
| 1:1A:4226:G:O2'    | 1:1A:4227:U:H5'    | 2.02                     | 0.60              |
| 1:1A:4956:A:O2'    | 1:1A:4957:C:H5'    | 2.01                     | 0.60              |
| 8:1H:138:ARG:NH1   | 8:1H:170:SER:HA    | 2.17                     | 0.60              |
| 10:2B:115:LEU:HD12 | 10:2B:116:ALA:N    | 2.16                     | 0.60              |
| 10:2B:265:LEU:HD12 | 10:2B:265:LEU:O    | 2.01                     | 0.60              |
| 12:2D:58:GLU:OE2   | 12:2D:161:GLY:HA3  | 2.01                     | 0.60              |
| 13:2E:31:ASP:HA    | 13:2E:34:THR:CG2   | 2.32                     | 0.60              |
| 14:2F:33:ILE:HG22  | 14:2F:37:LYS:HZ2   | 1.67                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:2S:53:ASP:OD2  | 27:2S:115:ARG:NH2  | 2.35                     | 0.60              |
| 47:2m:213:G:O2'   | 47:2m:214:U:OP1    | 2.19                     | 0.60              |
| 47:2m:1094:C:O2'  | 47:2m:1095:U:H5'   | 2.02                     | 0.60              |
| 47:2m:1112:U:O2   | 47:2m:1113:A:O2'   | 2.17                     | 0.60              |
| 47:2m:1283:C:C5   | 72:3J:104:VAL:HG11 | 2.37                     | 0.60              |
| 47:2m:1377:U:O2   | 47:2m:1379:A:H5'   | 2.02                     | 0.60              |
| 47:2m:1562:C:H4'  | 61:20:120:GLY:N    | 2.16                     | 0.60              |
| 50:2p:80:PRO:HG2  | 50:2p:83:SER:CB    | 2.32                     | 0.60              |
| 50:2p:172:VAL:O   | 50:2p:173:ARG:HD3  | 2.02                     | 0.60              |
| 54:2t:105:ASP:OD1 | 54:2t:106:SER:N    | 2.34                     | 0.60              |
| 68:3F:14:HIS:O    | 68:3F:305:ASN:HB3  | 2.02                     | 0.60              |
| 76:3N:13:MET:CE   | 76:3N:15:ASN:HB3   | 2.31                     | 0.60              |
| 1:1A:163:A:H2'    | 1:1A:164:G:C8      | 2.37                     | 0.60              |
| 1:1A:483:G:H3'    | 1:1A:484:U:C5'     | 2.31                     | 0.60              |
| 1:1A:1307:A:H2'   | 1:1A:1308:C:C6     | 2.37                     | 0.60              |
| 1:1A:1326:A:H2'   | 1:1A:1327:C:C6     | 2.37                     | 0.60              |
| 1:1A:1431:C:H2'   | 1:1A:1432:G:O4'    | 2.02                     | 0.60              |
| 1:1A:1479:G:H2'   | 1:1A:1480:C:C6     | 2.37                     | 0.60              |
| 1:1A:1958:A:O2'   | 1:1A:2025:A:N1     | 2.35                     | 0.60              |
| 1:1A:3592:G:H2'   | 1:1A:3593:C:O4'    | 2.01                     | 0.60              |
| 1:1A:4173:G:H2'   | 1:1A:4174:U:C6     | 2.36                     | 0.60              |
| 1:1A:4254:G:H2'   | 1:1A:4254:G:N3     | 2.17                     | 0.60              |
| 6:1F:117:THR:O    | 6:1F:121:ARG:HG3   | 2.02                     | 0.60              |
| 12:2D:34:PHE:HD2  | 12:2D:89:VAL:HG23  | 1.66                     | 0.60              |
| 46:2l:91:LYS:HA   | 46:2l:124:LEU:CD2  | 2.31                     | 0.60              |
| 47:2m:694:G:N1    | 47:2m:738:C:H4'    | 2.17                     | 0.60              |
| 47:2m:905:C:H2'   | 47:2m:906:U:N1     | 2.17                     | 0.60              |
| 47:2m:916:A:C5    | 73:3K:73:ARG:HD3   | 2.37                     | 0.60              |
| 47:2m:1309:C:H2'  | 47:2m:1310:U:C6    | 2.37                     | 0.60              |
| 47:2m:1425:G:O2'  | 47:2m:1426:U:OP1   | 2.19                     | 0.60              |
| 49:2o:193:ILE:O   | 49:2o:197:ILE:HG12 | 2.01                     | 0.60              |
| 50:2p:132:LYS:HB3 | 50:2p:189:MET:SD   | 2.42                     | 0.60              |
| 59:2y:73:LEU:HD13 | 59:2y:76:GLU:CD    | 2.27                     | 0.60              |
| 60:2z:28:PHE:HZ   | 61:20:45:LEU:HD21  | 1.64                     | 0.60              |
| 63:3A:40:ASP:OD1  | 63:3A:43:THR:N     | 2.28                     | 0.60              |
| 76:3N:50:THR:CG2  | 76:3N:55:ILE:HD11  | 2.32                     | 0.60              |
| 1:1A:1349:G:O3'   | 19:2K:20:SER:HB2   | 2.01                     | 0.60              |
| 1:1A:1365:C:H2'   | 1:1A:1366:G:C5'    | 2.32                     | 0.60              |
| 1:1A:1369:C:OP2   | 1:1A:1370:G:O2'    | 2.07                     | 0.60              |
| 1:1A:1661:C:O2'   | 1:1A:1662:C:H5'    | 2.01                     | 0.60              |
| 1:1A:2565:A:N7    | 1:1A:2566:G:H1'    | 2.17                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:1A:3920:U:H2'     | 1:1A:3921:U:C6     | 2.37                     | 0.60              |
| 1:1A:4323:A:C6      | 7:1G:153:THR:HG21  | 2.36                     | 0.60              |
| 1:1A:5024:C:N4      | 1:1A:5029:C:O4'    | 2.34                     | 0.60              |
| 5:1E:92:TYR:HB2     | 5:1E:159:VAL:HB    | 1.83                     | 0.60              |
| 10:2B:137[B]:ARG:CD | 10:2B:146:LEU:HD11 | 2.32                     | 0.60              |
| 21:2M:161:ARG:HD2   | 21:2M:164:LYS:HB2  | 1.84                     | 0.60              |
| 22:2N:118:GLU:OE2   | 22:2N:122:LYS:HE2  | 2.02                     | 0.60              |
| 25:2Q:52:THR:HG22   | 25:2Q:54:LEU:N     | 2.17                     | 0.60              |
| 39:2e:66:VAL:HG13   | 39:2e:66:VAL:O     | 1.99                     | 0.60              |
| 43:2i:99:ARG:HG2    | 43:2i:99:ARG:HH11  | 1.66                     | 0.60              |
| 47:2m:77:A:C2       | 70:3H:175:LYS:HD3  | 2.37                     | 0.60              |
| 47:2m:1114:U:O2'    | 47:2m:1115:U:H2'   | 2.02                     | 0.60              |
| 47:2m:1284:A:OP1    | 47:2m:1286:G:H4'   | 2.01                     | 0.60              |
| 47:2m:1419:C:H5'    | 61:20:125:PRO:O    | 2.02                     | 0.60              |
| 50:2p:92:ALA:HB3    | 50:2p:198:ILE:HD11 | 1.83                     | 0.60              |
| 59:2y:62:GLN:OE1    | 59:2y:62:GLN:N     | 2.35                     | 0.60              |
| 68:3F:8:ARG:HD2     | 68:3F:8:ARG:C      | 2.25                     | 0.60              |
| 70:3H:181:THR:HG22  | 70:3H:184:VAL:H    | 1.65                     | 0.60              |
| 72:3J:49:LEU:HD12   | 72:3J:111:VAL:HG22 | 1.83                     | 0.60              |
| 1:1A:178:C:H2'      | 1:1A:179:G:C8      | 2.37                     | 0.59              |
| 1:1A:518:G:H1       | 1:1A:643:C:H3'     | 1.66                     | 0.59              |
| 1:1A:2264:C:O2'     | 1:1A:2265:G:H5'    | 2.02                     | 0.59              |
| 1:1A:2329:U:O2'     | 1:1A:2330:G:H5'    | 2.01                     | 0.59              |
| 1:1A:4109:G:O2'     | 1:1A:4110:C:O5'    | 2.19                     | 0.59              |
| 1:1A:5021:C:H2'     | 1:1A:5022:U:O4'    | 2.02                     | 0.59              |
| 11:2C:106:GLN:OE1   | 11:2C:106:GLN:HA   | 2.00                     | 0.59              |
| 14:2F:125:ILE:HD13  | 14:2F:146:LEU:O    | 2.02                     | 0.59              |
| 16:2H:60:VAL:CG2    | 16:2H:134:LEU:HB2  | 2.30                     | 0.59              |
| 26:2R:52:LEU:HD13   | 26:2R:53:ARG:N     | 2.17                     | 0.59              |
| 46:2l:208:SER:HB3   | 46:2l:212:LYS:NZ   | 2.17                     | 0.59              |
| 47:2m:166:A:H5''    | 70:3H:112:VAL:HG21 | 1.84                     | 0.59              |
| 47:2m:195:C:H2'     | 47:2m:196:C:H6     | 1.67                     | 0.59              |
| 47:2m:534:G:H2'     | 47:2m:535:G:H8     | 1.64                     | 0.59              |
| 47:2m:1263:U:O2'    | 67:3E:27:ARG:HG3   | 2.02                     | 0.59              |
| 47:2m:1507:G:H1     | 80:3R:90:LYS:CA    | 2.13                     | 0.59              |
| 59:2y:87:GLU:HG2    | 59:2y:88:VAL:HG13  | 1.84                     | 0.59              |
| 64:3B:57:VAL:HG21   | 64:3B:115:ILE:HG23 | 1.83                     | 0.59              |
| 72:3J:25:ALA:CB     | 72:3J:31:LEU:HD11  | 2.32                     | 0.59              |
| 77:3O:57:LYS:HA     | 77:3O:60:LYS:CG    | 2.32                     | 0.59              |
| 78:3P:59:CYS:SG     | 78:3P:61:THR:OG1   | 2.60                     | 0.59              |
| 1:1A:209:U:O4       | 1:1A:211:G:H1'     | 2.03                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:494:U:H1'    | 1:1A:660:A:N1      | 2.16                     | 0.59              |
| 1:1A:1175:A:H4'   | 7:1G:268:ARG:HH21  | 1.66                     | 0.59              |
| 1:1A:1346:C:H2'   | 1:1A:1347:G:H8     | 1.67                     | 0.59              |
| 1:1A:1481:C:H41   | 37:2c:4:ARG:HG3    | 1.67                     | 0.59              |
| 1:1A:2103:G:N3    | 1:1A:2103:G:H2'    | 2.17                     | 0.59              |
| 1:1A:2376:A:H2'   | 1:1A:2377:C:C6     | 2.37                     | 0.59              |
| 1:1A:2675:G:N7    | 31:2W:32:LYS:HG3   | 2.17                     | 0.59              |
| 1:1A:4303:C:H2'   | 1:1A:4305:G:H8     | 1.66                     | 0.59              |
| 1:1A:4926:C:H2'   | 1:1A:4927:G:O4'    | 2.02                     | 0.59              |
| 7:1G:289:ARG:O    | 7:1G:293:ARG:HG2   | 2.02                     | 0.59              |
| 13:2E:3:GLN:OE1   | 13:2E:7:GLU:HB2    | 2.02                     | 0.59              |
| 46:2l:59:PRO:HB3  | 46:2l:171:HIS:N    | 2.17                     | 0.59              |
| 47:2m:189:U:O2    | 47:2m:211:G:N1     | 2.19                     | 0.59              |
| 47:2m:336:A:H2'   | 47:2m:337:C:C6     | 2.36                     | 0.59              |
| 47:2m:505:G:O2'   | 47:2m:506:G:H5'    | 2.02                     | 0.59              |
| 47:2m:902:G:H1    | 47:2m:903:A:HO2'   | 1.42                     | 0.59              |
| 47:2m:1103:C:H2'  | 47:2m:1104:G:H8    | 1.67                     | 0.59              |
| 47:2m:1622:U:H5'' | 60:2z:120:HIS:HB3  | 1.84                     | 0.59              |
| 51:2q:125:LYS:HB3 | 51:2q:142:HIS:HB3  | 1.83                     | 0.59              |
| 52:2r:139:VAL:HA  | 66:3D:63:ARG:HH12  | 1.66                     | 0.59              |
| 52:2r:195:GLU:HG3 | 52:2r:198:ARG:HH22 | 1.67                     | 0.59              |
| 61:20:52:TRP:O    | 61:20:55:THR:HG23  | 2.02                     | 0.59              |
| 63:3A:68:SER:HA   | 63:3A:71:ARG:NH1   | 2.16                     | 0.59              |
| 68:3F:67:SER:H    | 68:3F:82:SER:HA    | 1.66                     | 0.59              |
| 70:3H:222:GLU:HA  | 70:3H:225:GLN:OE1  | 2.02                     | 0.59              |
| 1:1A:149:A:H5''   | 1:1A:151:G:O4'     | 2.02                     | 0.59              |
| 1:1A:717:U:H2'    | 1:1A:718:C:C6      | 2.37                     | 0.59              |
| 1:1A:1174:G:H2'   | 1:1A:1175:A:C8     | 2.37                     | 0.59              |
| 1:1A:2711:G:H3'   | 1:1A:2712:G:C5'    | 2.32                     | 0.59              |
| 1:1A:3772:U:H1'   | 1:1A:3776:G:C6     | 2.36                     | 0.59              |
| 1:1A:3944:G:O6    | 1:1A:4069:U:O4     | 2.20                     | 0.59              |
| 1:1A:4220:A:OP2   | 22:2N:2:THR:N      | 2.35                     | 0.59              |
| 4:1D:115:CYS:O    | 4:1D:164:ALA:HA    | 2.01                     | 0.59              |
| 6:1F:124:ILE:HG21 | 6:1F:264:TYR:OH    | 2.02                     | 0.59              |
| 6:1F:347:HIS:O    | 6:1F:351:VAL:HG13  | 2.03                     | 0.59              |
| 12:2D:180:GLU:CG  | 12:2D:184:MET:HE1  | 2.26                     | 0.59              |
| 26:2R:93:ASN:HB2  | 26:2R:95:THR:HG22  | 1.84                     | 0.59              |
| 46:2l:108:ASP:OD1 | 46:2l:109:ALA:N    | 2.35                     | 0.59              |
| 47:2m:1330:G:O6   | 47:2m:1492:U:H2'   | 2.02                     | 0.59              |
| 47:2m:1338:G:O2'  | 47:2m:1339:U:H5'   | 2.02                     | 0.59              |
| 47:2m:1518:C:C5'  | 47:2m:1519:U:H5''  | 2.30                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:2r:167:LYS:HA  | 77:3O:71:ALA:HB1   | 1.84                     | 0.59              |
| 53:2s:58:LYS:HE3  | 53:2s:90:LYS:CE    | 2.33                     | 0.59              |
| 60:2z:23:ARG:O    | 60:2z:55:ARG:HD3   | 2.01                     | 0.59              |
| 76:3N:114:MET:O   | 76:3N:122:LYS:NZ   | 2.29                     | 0.59              |
| 1:1A:2:G:O2'      | 1:1A:3:C:H5'       | 2.02                     | 0.59              |
| 1:1A:184:U:O2     | 1:1A:184:U:H2'     | 2.01                     | 0.59              |
| 1:1A:1604:G:H2'   | 1:1A:1605:G:C8     | 2.38                     | 0.59              |
| 1:1A:1703:C:H5''  | 1:1A:1704:C:C5     | 2.38                     | 0.59              |
| 1:1A:2480:G:O2'   | 1:1A:2481:G:H5'    | 2.02                     | 0.59              |
| 1:1A:4953:G:H2'   | 1:1A:4954:G:C8     | 2.37                     | 0.59              |
| 5:1E:161:ARG:HG2  | 5:1E:184:GLN:HA    | 1.82                     | 0.59              |
| 9:2A:114:LEU:HD21 | 9:2A:121:THR:CG2   | 2.32                     | 0.59              |
| 23:2O:49:VAL:HG21 | 23:2O:57:GLY:HA3   | 1.84                     | 0.59              |
| 29:2U:36:GLY:HA3  | 29:2U:40:HIS:CE1   | 2.37                     | 0.59              |
| 31:2W:28:VAL:HG13 | 31:2W:33:GLN:HB3   | 1.83                     | 0.59              |
| 47:2m:301:A:O2'   | 54:2t:73:THR:HG22  | 2.02                     | 0.59              |
| 47:2m:367:U:H4'   | 47:2m:371:A:C8     | 2.37                     | 0.59              |
| 47:2m:528:A:H2'   | 47:2m:529:A:C8     | 2.37                     | 0.59              |
| 47:2m:745:C:H2'   | 47:2m:796:G:N2     | 2.17                     | 0.59              |
| 47:2m:1258:A:C2   | 47:2m:1663:A:H2'   | 2.37                     | 0.59              |
| 47:2m:1571:G:H2'  | 47:2m:1572:C:C6    | 2.38                     | 0.59              |
| 49:2o:81:PHE:O    | 49:2o:106:THR:HG23 | 2.02                     | 0.59              |
| 50:2p:76:ARG:HB2  | 55:2u:22:VAL:HG11  | 1.83                     | 0.59              |
| 51:2q:102:ILE:CD1 | 51:2q:239:PRO:HD3  | 2.30                     | 0.59              |
| 58:2x:39:LEU:CD1  | 58:2x:51:LEU:HD21  | 2.31                     | 0.59              |
| 58:2x:93:VAL:HG11 | 58:2x:109:LYS:HZ3  | 1.68                     | 0.59              |
| 62:21:28:ASN:HD21 | 62:21:31:SER:HG    | 1.44                     | 0.59              |
| 69:3G:77:SER:OG   | 69:3G:80:GLU:HB2   | 2.03                     | 0.59              |
| 69:3G:142:LYS:CD  | 69:3G:153:GLY:HA3  | 2.31                     | 0.59              |
| 71:3I:28:GLU:HG3  | 71:3I:40:LYS:CE    | 2.31                     | 0.59              |
| 72:3J:49:LEU:HD21 | 72:3J:123:VAL:HG11 | 1.84                     | 0.59              |
| 1:1A:108:A:H4'    | 1:1A:109:G:OP1     | 2.02                     | 0.59              |
| 1:1A:382:G:O2'    | 1:1A:407:A:N6      | 2.30                     | 0.59              |
| 1:1A:1440:U:H3    | 1:1A:2105:A:H2     | 1.51                     | 0.59              |
| 1:1A:1508:A:OP1   | 6:1F:110:ARG:NH2   | 2.35                     | 0.59              |
| 1:1A:2516:G:OP2   | 35:2a:37:LYS:NZ    | 2.26                     | 0.59              |
| 1:1A:4260:U:H2'   | 1:1A:4261:C:C6     | 2.38                     | 0.59              |
| 1:1A:4699:U:H1'   | 1:1A:4700:A:H5''   | 1.83                     | 0.59              |
| 1:1A:4902:C:H2'   | 1:1A:4903:G:H8     | 1.67                     | 0.59              |
| 9:2A:39:GLN:HA    | 9:2A:39:GLN:HE21   | 1.66                     | 0.59              |
| 27:2S:51:LYS:HE3  | 27:2S:71:VAL:O     | 2.02                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:560:A:O5'    | 71:3I:174:LYS:HG3  | 2.03                     | 0.59              |
| 47:2m:570:C:C2     | 47:2m:571:U:C6     | 2.90                     | 0.59              |
| 47:2m:615:C:H2'    | 47:2m:616:A:O4'    | 2.02                     | 0.59              |
| 47:2m:1377:U:H3'   | 48:2n:102:ARG:NH2  | 2.16                     | 0.59              |
| 47:2m:1642:U:O2'   | 47:2m:1643:U:H5'   | 2.02                     | 0.59              |
| 47:2m:1678:A:H3'   | 47:2m:1679:A:C8    | 2.37                     | 0.59              |
| 53:2s:111:LYS:HD3  | 53:2s:112:ASN:N    | 2.16                     | 0.59              |
| 54:2t:119:LEU:CD2  | 54:2t:153:LYS:HD3  | 2.33                     | 0.59              |
| 54:2t:129:LEU:CB   | 54:2t:133:GLU:HB2  | 2.30                     | 0.59              |
| 56:2v:111:VAL:HG12 | 56:2v:140:PHE:HB2  | 1.83                     | 0.59              |
| 57:2w:56:LEU:HG    | 57:2w:60:LEU:CD2   | 2.32                     | 0.59              |
| 57:2w:58:LYS:HD2   | 57:2w:61:ARG:HH12  | 1.68                     | 0.59              |
| 57:2w:74:GLU:OE1   | 57:2w:74:GLU:N     | 2.36                     | 0.59              |
| 59:2y:20:TYR:CE2   | 59:2y:38:ILE:HG21  | 2.38                     | 0.59              |
| 60:2z:15:VAL:HG12  | 60:2z:16:LEU:HD12  | 1.84                     | 0.59              |
| 61:20:14:PHE:CE1   | 61:20:134:ILE:HD11 | 2.38                     | 0.59              |
| 61:20:131:LEU:O    | 61:20:134:ILE:HG13 | 2.01                     | 0.59              |
| 61:20:133:ARG:NH1  | 61:20:134:ILE:HG22 | 2.13                     | 0.59              |
| 65:3C:49:ALA:HB2   | 74:3L:117:ARG:HH21 | 1.68                     | 0.59              |
| 69:3G:88:ILE:HD13  | 69:3G:94:ILE:HD11  | 1.85                     | 0.59              |
| 70:3H:199:THR:HG22 | 70:3H:203:LYS:NZ   | 2.18                     | 0.59              |
| 76:3N:35:VAL:O     | 76:3N:40:ILE:HD11  | 2.02                     | 0.59              |
| 1:1A:313:U:O2'     | 1:1A:314:G:H5'     | 2.01                     | 0.59              |
| 1:1A:1077:C:OP1    | 1:1A:1215:C:H2'    | 2.03                     | 0.59              |
| 1:1A:1739:G:H2'    | 1:1A:1740:C:C6     | 2.38                     | 0.59              |
| 1:1A:1739:G:O2'    | 1:1A:1740:C:H5'    | 2.03                     | 0.59              |
| 1:1A:4147:G:H2'    | 1:1A:4148:C:C6     | 2.37                     | 0.59              |
| 2:1B:16:A:H2'      | 2:1B:17:C:C6       | 2.37                     | 0.59              |
| 11:2C:91:LYS:HG3   | 11:2C:183:GLU:OE2  | 2.02                     | 0.59              |
| 30:2V:68:ARG:O     | 30:2V:72:ILE:HG12  | 2.01                     | 0.59              |
| 39:2e:10:ASP:HA    | 39:2e:13:LEU:HD23  | 1.84                     | 0.59              |
| 46:2I:119:GLN:HA   | 46:2I:122:ARG:HH21 | 1.67                     | 0.59              |
| 47:2m:1471:C:H2'   | 47:2m:1472:C:C6    | 2.37                     | 0.59              |
| 47:2m:1867:U:H4'   | 47:2m:1868:U:H5'   | 1.84                     | 0.59              |
| 50:2p:47:GLU:HB3   | 50:2p:85:GLU:OE2   | 2.02                     | 0.59              |
| 51:2q:112:HIS:NE2  | 51:2q:237:SER:O    | 2.35                     | 0.59              |
| 53:2s:6:ALA:HB3    | 53:2s:28:LEU:CD2   | 2.33                     | 0.59              |
| 59:2y:77:GLU:OE1   | 59:2y:78:ARG:N     | 2.34                     | 0.59              |
| 60:2z:26:ILE:HG22  | 60:2z:54:LYS:O     | 2.02                     | 0.59              |
| 68:3F:70:VAL:C     | 68:3F:71:ILE:HD12  | 2.28                     | 0.59              |
| 1:1A:1241:C:H5     | 30:2V:118:LEU:HD23 | 1.67                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1552:G:H1'   | 1:1A:1575:A:N6     | 2.18                     | 0.59              |
| 1:1A:1766:A:N6    | 57:2w:10:ARG:HD2   | 2.16                     | 0.59              |
| 1:1A:2029:A:O2'   | 1:1A:2030:A:H5'    | 2.02                     | 0.59              |
| 1:1A:2587:A:O2'   | 1:1A:2588:C:O4'    | 2.12                     | 0.59              |
| 1:1A:3859:G:OP1   | 18:2J:141:SER:HB3  | 2.02                     | 0.59              |
| 1:1A:3880:G:O2'   | 1:1A:3881:G:H5'    | 2.02                     | 0.59              |
| 1:1A:3912:U:O2'   | 1:1A:3913:G:H5'    | 2.03                     | 0.59              |
| 1:1A:4110:C:H4'   | 1:1A:4111:U:OP1    | 2.03                     | 0.59              |
| 1:1A:4131:G:O2'   | 1:1A:4132:C:H5'    | 2.02                     | 0.59              |
| 1:1A:4152:G:O2'   | 1:1A:4153:C:H5'    | 2.03                     | 0.59              |
| 1:1A:4271:A:O2'   | 1:1A:4272:G:H5'    | 2.02                     | 0.59              |
| 1:1A:4316:G:C2'   | 1:1A:4317:A:H5'    | 2.33                     | 0.59              |
| 1:1A:4744:A:H2'   | 1:1A:4745:G:H8     | 1.68                     | 0.59              |
| 1:1A:4772:C:H2'   | 1:1A:4773:C:C5     | 2.37                     | 0.59              |
| 1:1A:4874:A:H2    | 17:2I:179:LYS:HG3  | 1.64                     | 0.59              |
| 1:1A:4957:C:H2'   | 1:1A:4958:C:H6     | 1.67                     | 0.59              |
| 1:1A:5064:G:O2'   | 1:1A:5065:U:H5'    | 2.02                     | 0.59              |
| 2:1B:46:C:OP1     | 7:1G:158:LYS:HG3   | 2.03                     | 0.59              |
| 3:1C:123:U:C5     | 3:1C:124:U:H1'     | 2.37                     | 0.59              |
| 39:2e:68:GLU:OE1  | 39:2e:68:GLU:N     | 2.36                     | 0.59              |
| 47:2m:102:A:H4'   | 47:2m:104:A:C8     | 2.38                     | 0.59              |
| 47:2m:845:G:H2'   | 47:2m:846:G:O4'    | 2.02                     | 0.59              |
| 47:2m:1398:G:H1'  | 68:3F:63:SER:HB2   | 1.85                     | 0.59              |
| 47:2m:1510:G:O2'  | 47:2m:1511:U:H5'   | 2.02                     | 0.59              |
| 59:2y:60:ARG:HG3  | 59:2y:63:ARG:HE    | 1.67                     | 0.59              |
| 64:3B:11:ARG:O    | 64:3B:14:ARG:HG3   | 2.02                     | 0.59              |
| 65:3C:45:VAL:HG21 | 65:3C:64:LEU:CD1   | 2.31                     | 0.59              |
| 69:3G:74:LYS:HG3  | 69:3G:74:LYS:O     | 2.03                     | 0.59              |
| 70:3H:23:LYS:HD3  | 70:3H:41:LEU:CA    | 2.33                     | 0.59              |
| 72:3J:89:VAL:CG2  | 72:3J:109:VAL:HG11 | 2.31                     | 0.59              |
| 77:3O:73:VAL:O    | 77:3O:79:ILE:HB    | 2.03                     | 0.59              |
| 1:1A:1308:C:H2'   | 1:1A:1309:C:C6     | 2.38                     | 0.59              |
| 1:1A:1998:A:H2'   | 1:1A:1999:A:C2     | 2.38                     | 0.59              |
| 1:1A:3963:A:H8    | 1:1A:3965:A:OP2    | 1.85                     | 0.59              |
| 1:1A:4637:G:O2'   | 1:1A:4638:U:H5'    | 2.02                     | 0.59              |
| 5:1E:206:PRO:HG2  | 5:1E:209:GLN:HG3   | 1.84                     | 0.59              |
| 13:2E:24:ILE:HD12 | 13:2E:40:LEU:HG    | 1.84                     | 0.59              |
| 16:2H:103:GLU:OE2 | 16:2H:118:SER:OG   | 2.13                     | 0.59              |
| 28:2T:104:PRO:O   | 28:2T:108:ARG:HG2  | 2.02                     | 0.59              |
| 46:2I:29:LEU:CD2  | 46:2I:173:LYS:HB3  | 2.31                     | 0.59              |
| 46:2I:50:SER:HA   | 46:2I:159:MET:SD   | 2.42                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:2l:88:GLU:H     | 46:2l:88:GLU:CD   | 2.11                     | 0.59              |
| 47:2m:996:A:H5''   | 73:3K:7:PRO:CD    | 2.33                     | 0.59              |
| 47:2m:1310:U:O5'   | 72:3J:36:ARG:NH2  | 2.36                     | 0.59              |
| 47:2m:1419:C:H4'   | 61:20:128:GLN:HG3 | 1.85                     | 0.59              |
| 49:2o:33:VAL:HG21  | 49:2o:67:PHE:CZ   | 2.38                     | 0.59              |
| 52:2r:98:GLU:O     | 52:2r:102:LEU:HG  | 2.03                     | 0.59              |
| 65:3C:45:VAL:HG21  | 65:3C:64:LEU:HB3  | 1.83                     | 0.59              |
| 68:3F:81:GLY:CA    | 68:3F:87:LEU:HD23 | 2.33                     | 0.59              |
| 1:1A:424:U:H2'     | 1:1A:425:U:C6     | 2.38                     | 0.59              |
| 1:1A:452:A:H4'     | 1:1A:453:G:C5'    | 2.27                     | 0.59              |
| 1:1A:967:C:C2'     | 1:1A:968:C:H5''   | 2.33                     | 0.59              |
| 1:1A:1175:A:H2     | 1:1A:1185:G:H22   | 1.51                     | 0.59              |
| 1:1A:1182:C:H3'    | 1:1A:1182:C:O2    | 2.03                     | 0.59              |
| 1:1A:1697:G:O2'    | 1:1A:1698:C:H5'   | 2.03                     | 0.59              |
| 1:1A:2078:C:OP1    | 33:2Y:64:LYS:HG2  | 2.02                     | 0.59              |
| 8:1H:130:LYS:N     | 8:1H:130:LYS:HD2  | 2.18                     | 0.59              |
| 13:2E:67:LYS:C     | 13:2E:68:ILE:HD13 | 2.28                     | 0.59              |
| 16:2H:126:THR:HG23 | 16:2H:127:TYR:CD2 | 2.38                     | 0.59              |
| 20:2L:176:ARG:NH2  | 47:2m:909:G:H5'   | 2.17                     | 0.59              |
| 33:2Y:86:GLU:OE2   | 33:2Y:114:ARG:NH2 | 2.31                     | 0.59              |
| 47:2m:1106:C:O2'   | 47:2m:1107:G:H5'  | 2.02                     | 0.59              |
| 47:2m:1223:A:H2'   | 47:2m:1224:G:O4'  | 2.03                     | 0.59              |
| 47:2m:1255:G:H5'   | 47:2m:1256:G:O5'  | 2.03                     | 0.59              |
| 47:2m:1277:C:N4    | 47:2m:1320:G:O6   | 2.32                     | 0.59              |
| 47:2m:1533:A:N3    | 47:2m:1536:G:O2'  | 2.24                     | 0.59              |
| 47:2m:1678:A:H3'   | 47:2m:1679:A:H8   | 1.68                     | 0.59              |
| 48:2n:80:ARG:O     | 48:2n:84:GLN:HG3  | 2.03                     | 0.59              |
| 50:2p:65:ARG:O     | 50:2p:68:GLU:HG2  | 2.03                     | 0.59              |
| 51:2q:42:LEU:CG    | 51:2q:46:ILE:HD11 | 2.29                     | 0.59              |
| 51:2q:60:GLU:HA    | 51:2q:63:LYS:HG2  | 1.84                     | 0.59              |
| 53:2s:64:VAL:HG12  | 53:2s:65:PRO:HD2  | 1.85                     | 0.59              |
| 53:2s:144:ILE:HD12 | 53:2s:144:ILE:N   | 2.18                     | 0.59              |
| 53:2s:149:ASP:OD1  | 53:2s:151:SER:N   | 2.29                     | 0.59              |
| 54:2t:125:LYS:HB3  | 54:2t:128:LYS:NZ  | 2.18                     | 0.59              |
| 60:2z:84:LEU:HD22  | 60:2z:95:TYR:CB   | 2.33                     | 0.59              |
| 61:20:113:VAL:HG22 | 61:20:121:ARG:HB3 | 1.84                     | 0.59              |
| 71:3I:65:GLU:OE1   | 71:3I:71:LEU:HD21 | 2.03                     | 0.59              |
| 74:3L:85:CYS:HB2   | 74:3L:124:MET:CE  | 2.33                     | 0.59              |
| 1:1A:137:G:O2'     | 1:1A:138:G:O4'    | 2.21                     | 0.59              |
| 1:1A:184:U:C5      | 1:1A:254:G:H2'    | 2.38                     | 0.59              |
| 1:1A:966:A:O2'     | 1:1A:967:C:H5'    | 2.03                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:978:G:H2'    | 1:1A:979:C:C6      | 2.38                     | 0.59              |
| 1:1A:1450:C:H2'   | 1:1A:1451:G:O4'    | 2.03                     | 0.59              |
| 1:1A:1807:C:O2'   | 1:1A:1808:C:H5'    | 2.02                     | 0.59              |
| 1:1A:2611:A:C5'   | 1:1A:2688:G:H4'    | 2.33                     | 0.59              |
| 1:1A:4082:G:O2'   | 1:1A:4083:U:H5'    | 2.03                     | 0.59              |
| 6:1F:348:LYS:O    | 6:1F:351:VAL:HG22  | 2.03                     | 0.59              |
| 8:1H:108:LYS:HG3  | 8:1H:108:LYS:O     | 2.02                     | 0.59              |
| 12:2D:208:LYS:HG3 | 12:2D:209:TRP:N    | 2.18                     | 0.59              |
| 23:2O:19:LEU:CB   | 23:2O:74:SER:O     | 2.45                     | 0.59              |
| 25:2Q:101:ARG:C   | 25:2Q:105:ARG:HG2  | 2.28                     | 0.59              |
| 46:2l:48:ARG:CG   | 46:2l:49:PHE:H     | 2.15                     | 0.59              |
| 47:2m:96:C:H1'    | 47:2m:474:G:H5'    | 1.83                     | 0.59              |
| 47:2m:465:A:H5'   | 47:2m:466:G:C8     | 2.38                     | 0.59              |
| 47:2m:1170:A:H4'  | 47:2m:1171:G:OP1   | 2.03                     | 0.59              |
| 47:2m:1539:U:H5'  | 61:20:45:LEU:O     | 2.02                     | 0.59              |
| 47:2m:1673:U:H5'' | 58:2x:78:VAL:HG23  | 1.85                     | 0.59              |
| 47:2m:1863:A:H1'  | 65:3C:79:ILE:CD1   | 2.33                     | 0.59              |
| 51:2q:151:ASP:OD2 | 51:2q:153:LEU:HB2  | 2.03                     | 0.59              |
| 55:2u:52:LEU:HD21 | 55:2u:58:VAL:HG13  | 1.84                     | 0.59              |
| 68:3F:17:TRP:CD1  | 68:3F:303:THR:HA   | 2.38                     | 0.59              |
| 1:1A:2635:U:O2'   | 1:1A:2636:U:H5'    | 2.03                     | 0.58              |
| 1:1A:2890:C:O2'   | 1:1A:2891:U:H5'    | 2.03                     | 0.58              |
| 1:1A:4646:U:OP1   | 20:2L:58:HIS:HA    | 2.03                     | 0.58              |
| 1:1A:4691:A:O3'   | 11:2C:71:ARG:HD3   | 2.03                     | 0.58              |
| 1:1A:5054:C:O2    | 81:1A:5101:84D:O6  | 2.21                     | 0.58              |
| 3:1C:70:G:H22     | 3:1C:87:G:H1'      | 1.68                     | 0.58              |
| 10:2B:206:GLN:OE1 | 10:2B:206:GLN:HA   | 2.03                     | 0.58              |
| 13:2E:144:LYS:HD3 | 13:2E:146:ARG:O    | 2.03                     | 0.58              |
| 13:2E:164:ARG:NH1 | 13:2E:167:GLN:OE1  | 2.36                     | 0.58              |
| 47:2m:306:C:H2'   | 47:2m:307:G:C5     | 2.38                     | 0.58              |
| 47:2m:847:A:O2'   | 47:2m:848:U:OP1    | 2.21                     | 0.58              |
| 47:2m:1293:A:OP1  | 80:3R:138:ARG:NH2  | 2.36                     | 0.58              |
| 47:2m:1348:G:H2'  | 47:2m:1349:G:C8    | 2.38                     | 0.58              |
| 47:2m:1440:C:O2'  | 47:2m:1441:U:H5'   | 2.01                     | 0.58              |
| 52:2r:125:SER:O   | 52:2r:135:ARG:HG3  | 2.03                     | 0.58              |
| 52:2r:138:ALA:O   | 66:3D:63:ARG:NH1   | 2.36                     | 0.58              |
| 58:2x:8:GLN:HB3   | 58:2x:27:ARG:CZ    | 2.33                     | 0.58              |
| 58:2x:134:GLY:HA3 | 58:2x:140:ARG:HA   | 1.84                     | 0.58              |
| 68:3F:120:ILE:O   | 68:3F:131:LEU:HD13 | 2.03                     | 0.58              |
| 69:3G:104:ASP:OD2 | 69:3G:130:ILE:HD13 | 2.03                     | 0.58              |
| 1:1A:454:U:H2'    | 1:1A:455:C:O4'     | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1662:C:H2'   | 1:1A:1663:C:H6    | 1.67                     | 0.58              |
| 1:1A:4364:G:H4'   | 29:2U:58:MET:HG2  | 1.84                     | 0.58              |
| 4:1D:171:GLY:O    | 44:2j:68:ALA:HB2  | 2.03                     | 0.58              |
| 8:1H:203:ILE:HG22 | 8:1H:203:ILE:O    | 2.01                     | 0.58              |
| 12:2D:102:MET:HG3 | 12:2D:102:MET:O   | 2.01                     | 0.58              |
| 21:2M:70:LYS:HE2  | 21:2M:70:LYS:HA   | 1.84                     | 0.58              |
| 47:2m:636:C:H2'   | 47:2m:637:U:H6    | 1.68                     | 0.58              |
| 47:2m:1543:U:H4'  | 58:2x:43:GLU:CG   | 2.32                     | 0.58              |
| 47:2m:1779:G:H2'  | 47:2m:1780:G:N7   | 2.17                     | 0.58              |
| 51:2q:100:ARG:HB2 | 51:2q:114:ILE:CD1 | 2.33                     | 0.58              |
| 55:2u:37:ASP:HB2  | 55:2u:38:LYS:NZ   | 2.18                     | 0.58              |
| 58:2x:123:ASP:OD2 | 58:2x:125:ARG:NH2 | 2.30                     | 0.58              |
| 68:3F:232:GLY:HA3 | 68:3F:259:TRP:CZ2 | 2.38                     | 0.58              |
| 68:3F:242:SER:OG  | 68:3F:245:ARG:HB2 | 2.04                     | 0.58              |
| 1:1A:286:U:H2'    | 1:1A:287:U:C6     | 2.38                     | 0.58              |
| 1:1A:518:G:H1     | 1:1A:643:C:C3'    | 2.16                     | 0.58              |
| 1:1A:1504:G:H2'   | 1:1A:1505:C:C6    | 2.37                     | 0.58              |
| 1:1A:1759:G:H2'   | 1:1A:1760:G:H5'   | 1.84                     | 0.58              |
| 1:1A:1824:G:H2'   | 1:1A:1825:A:H8    | 1.67                     | 0.58              |
| 1:1A:1920:C:C3'   | 1:1A:1921:C:H5''  | 2.29                     | 0.58              |
| 1:1A:1961:G:H5'   | 1:1A:1962:A:OP1   | 2.02                     | 0.58              |
| 1:1A:2587:A:H3'   | 1:1A:2588:C:C6    | 2.38                     | 0.58              |
| 1:1A:4301:U:OP2   | 22:2N:87:LYS:NZ   | 2.36                     | 0.58              |
| 1:1A:4996:C:OP1   | 32:2X:32:ARG:NH1  | 2.31                     | 0.58              |
| 2:1B:4:U:H2'      | 2:1B:5:A:H8       | 1.68                     | 0.58              |
| 3:1C:81:C:H5'     | 36:2b:3:LYS:NZ    | 2.18                     | 0.58              |
| 11:2C:50:LYS:H    | 11:2C:50:LYS:HD2  | 1.69                     | 0.58              |
| 27:2S:2:LYS:HD3   | 27:2S:7:VAL:CG2   | 2.33                     | 0.58              |
| 47:2m:901:G:H2'   | 47:2m:902:G:O4'   | 2.03                     | 0.58              |
| 47:2m:1486:A:HO2' | 47:2m:1487:A:P    | 2.25                     | 0.58              |
| 47:2m:1526:G:H2'  | 47:2m:1526:G:N3   | 2.17                     | 0.58              |
| 48:2n:23:THR:OG1  | 48:2n:174:MET:HE1 | 2.03                     | 0.58              |
| 50:2p:33:GLY:O    | 50:2p:52:ALA:HA   | 2.03                     | 0.58              |
| 53:2s:15:LYS:NZ   | 53:2s:17:ASP:OD2  | 2.29                     | 0.58              |
| 53:2s:80:VAL:O    | 53:2s:84:GLU:HG2  | 2.03                     | 0.58              |
| 68:3F:11:LEU:HB3  | 68:3F:43:TRP:CH2  | 2.38                     | 0.58              |
| 68:3F:21:ILE:CG2  | 68:3F:31:ILE:HD11 | 2.32                     | 0.58              |
| 70:3H:55:GLY:O    | 70:3H:63:MET:HG2  | 2.03                     | 0.58              |
| 70:3H:148:SER:O   | 70:3H:149:LYS:HD2 | 2.03                     | 0.58              |
| 77:3O:47:LEU:CD1  | 77:3O:83:LEU:HD12 | 2.33                     | 0.58              |
| 77:3O:57:LYS:HA   | 77:3O:60:LYS:HD2  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:288:G:H2'    | 1:1A:289:C:C6      | 2.38                     | 0.58              |
| 1:1A:654:C:H5'    | 6:1F:268:ARG:NH2   | 2.19                     | 0.58              |
| 1:1A:963:G:OP2    | 9:2A:32:ARG:HD2    | 2.04                     | 0.58              |
| 1:1A:1364:U:OP2   | 14:2F:36:ARG:NH1   | 2.31                     | 0.58              |
| 1:1A:1613:A:H5''  | 4:1D:183:GLY:HA2   | 1.85                     | 0.58              |
| 1:1A:2020:U:H3'   | 1:1A:2021:G:H5''   | 1.85                     | 0.58              |
| 1:1A:2261:G:H5''  | 8:1H:112:MET:CE    | 2.32                     | 0.58              |
| 1:1A:2264:C:H2'   | 1:1A:2265:G:O4'    | 2.03                     | 0.58              |
| 1:1A:2570:U:O2'   | 1:1A:2571:C:H5'    | 2.04                     | 0.58              |
| 1:1A:2824:C:H2'   | 1:1A:2825:A:C8     | 2.38                     | 0.58              |
| 1:1A:3595:U:OP1   | 1:1A:3597:G:H1'    | 2.02                     | 0.58              |
| 1:1A:3870:C:H2'   | 1:1A:3871:A:H8     | 1.68                     | 0.58              |
| 1:1A:5004:C:O2'   | 1:1A:5005:G:H5'    | 2.03                     | 0.58              |
| 5:1E:17:LEU:HD21  | 5:1E:264:PHE:HD2   | 1.67                     | 0.58              |
| 6:1F:209:ILE:HB   | 6:1F:229:LEU:HD13  | 1.84                     | 0.58              |
| 12:2D:51:HIS:ND1  | 12:2D:137:SER:OG   | 2.36                     | 0.58              |
| 13:2E:119:TYR:CD2 | 60:2z:12:ILE:HG12  | 2.38                     | 0.58              |
| 18:2J:7:ASP:OD1   | 18:2J:7:ASP:N      | 2.36                     | 0.58              |
| 27:2S:82:ILE:HG22 | 27:2S:83:GLU:H     | 1.69                     | 0.58              |
| 46:2l:11:TYR:O    | 46:2l:12:GLU:HG2   | 2.01                     | 0.58              |
| 46:2l:63:PHE:O    | 46:2l:153:SER:OG   | 2.13                     | 0.58              |
| 46:2l:184:HIS:O   | 46:2l:185:LEU:HD23 | 2.04                     | 0.58              |
| 47:2m:45:A:O2'    | 47:2m:480:G:N2     | 2.37                     | 0.58              |
| 47:2m:687:C:O2'   | 53:2s:103:LYS:HE2  | 2.04                     | 0.58              |
| 47:2m:975:G:O2'   | 47:2m:976:G:H5'    | 2.03                     | 0.58              |
| 47:2m:1158:G:H5'' | 75:3M:76:SER:HB3   | 1.84                     | 0.58              |
| 47:2m:1235:G:H2'  | 47:2m:1236:G:C8    | 2.38                     | 0.58              |
| 47:2m:1299:A:H2'  | 47:2m:1300:U:H3'   | 1.86                     | 0.58              |
| 47:2m:1409:A:H4'  | 58:2x:26:LYS:HD3   | 1.86                     | 0.58              |
| 47:2m:1618:C:O2'  | 57:2w:50:ARG:NE    | 2.36                     | 0.58              |
| 47:2m:1748:G:N2   | 47:2m:1786:U:O2    | 2.27                     | 0.58              |
| 50:2p:95:GLY:HA2  | 50:2p:101:GLN:NE2  | 2.19                     | 0.58              |
| 50:2p:143:ARG:HG2 | 50:2p:143:ARG:O    | 2.02                     | 0.58              |
| 50:2p:177:LEU:CD2 | 50:2p:178:ARG:HG3  | 2.31                     | 0.58              |
| 61:20:112:MET:O   | 61:20:124:THR:HG23 | 2.02                     | 0.58              |
| 61:20:114:GLU:CD  | 61:20:124:THR:HG22 | 2.28                     | 0.58              |
| 65:3C:41:ILE:HG13 | 65:3C:68:TYR:CD2   | 2.38                     | 0.58              |
| 65:3C:89:ARG:HG2  | 65:3C:90:GLU:OE1   | 2.03                     | 0.58              |
| 68:3F:139:LYS:HG2 | 68:3F:140:TYR:H    | 1.69                     | 0.58              |
| 68:3F:301:GLY:CA  | 68:3F:307:VAL:HG22 | 2.33                     | 0.58              |
| 69:3G:133:TYR:HD1 | 69:3G:216:MET:HA   | 1.65                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:3H:162:LEU:HD12 | 70:3H:162:LEU:O    | 2.03                     | 0.58              |
| 71:3I:81:LEU:HD22  | 71:3I:86:VAL:HG21  | 1.84                     | 0.58              |
| 73:3K:33:VAL:O     | 73:3K:37:ILE:HG13  | 2.03                     | 0.58              |
| 1:1A:193:G:O2'     | 1:1A:194:C:H5'     | 2.04                     | 0.58              |
| 1:1A:1474:C:O2'    | 1:1A:1475:G:H5'    | 2.03                     | 0.58              |
| 1:1A:2736:G:O2'    | 1:1A:2737:C:H5'    | 2.03                     | 0.58              |
| 1:1A:4769:G:H2'    | 1:1A:4770:U:C5'    | 2.33                     | 0.58              |
| 8:1H:162:VAL:HG21  | 8:1H:175:VAL:HG11  | 1.85                     | 0.58              |
| 10:2B:105:GLU:OE1  | 10:2B:110:LYS:HB2  | 2.03                     | 0.58              |
| 16:2H:185:GLY:HA3  | 16:2H:194:ARG:HH12 | 1.67                     | 0.58              |
| 28:2T:22:LYS:HE2   | 28:2T:132:GLN:O    | 2.04                     | 0.58              |
| 46:2L:59:PRO:HB3   | 46:2L:171:HIS:H    | 1.68                     | 0.58              |
| 47:2m:832:G:O2'    | 47:2m:833:C:H5'    | 2.03                     | 0.58              |
| 51:2q:64:ILE:HD12  | 76:3N:17:LEU:HD23  | 1.86                     | 0.58              |
| 51:2q:179:ASN:HA   | 51:2q:231:GLY:H    | 1.69                     | 0.58              |
| 55:2u:57:TYR:HB3   | 55:2u:75:GLY:HA2   | 1.86                     | 0.58              |
| 59:2y:56:HIS:ND1   | 59:2y:59:LYS:HE2   | 2.18                     | 0.58              |
| 61:20:28:LEU:HD21  | 61:20:54:TYR:CE2   | 2.39                     | 0.58              |
| 64:3B:32:LEU:CD2   | 64:3B:34:THR:HG22  | 2.32                     | 0.58              |
| 65:3C:52:ASP:CG    | 74:3L:121:ARG:HD3  | 2.29                     | 0.58              |
| 68:3F:63:SER:HB3   | 68:3F:84:ASP:HB3   | 1.83                     | 0.58              |
| 70:3H:74:ARG:O     | 70:3H:75:LEU:HD23  | 2.03                     | 0.58              |
| 70:3H:120:ASP:HB2  | 70:3H:125:THR:CG2  | 2.33                     | 0.58              |
| 71:3I:28:GLU:HG3   | 71:3I:40:LYS:HD3   | 1.85                     | 0.58              |
| 72:3J:51:VAL:CG1   | 72:3J:109:VAL:HG23 | 2.34                     | 0.58              |
| 76:3N:111:LYS:O    | 76:3N:114:MET:HE3  | 2.03                     | 0.58              |
| 1:1A:334:A:O2'     | 1:1A:335:A:H5'     | 2.04                     | 0.58              |
| 1:1A:347:A:H2'     | 1:1A:348:G:C8      | 2.38                     | 0.58              |
| 1:1A:921:C:O2'     | 1:1A:922:C:H5'     | 2.04                     | 0.58              |
| 1:1A:1779:U:H2'    | 1:1A:1780:A:C8     | 2.39                     | 0.58              |
| 1:1A:2068:C:OP1    | 34:2Z:15:LYS:HE3   | 2.04                     | 0.58              |
| 1:1A:2350:U:H5''   | 1:1A:2351:C:H5''   | 1.85                     | 0.58              |
| 1:1A:4111:U:H3'    | 1:1A:4111:U:OP2    | 2.03                     | 0.58              |
| 1:1A:4364:G:C4'    | 29:2U:58:MET:HG2   | 2.33                     | 0.58              |
| 1:1A:4885:U:H2'    | 1:1A:4886:C:O4'    | 2.04                     | 0.58              |
| 3:1C:29:G:O2'      | 3:1C:30:U:H5'      | 2.04                     | 0.58              |
| 3:1C:51:U:H2'      | 3:1C:51:U:O2       | 2.02                     | 0.58              |
| 6:1F:134:PRO:CA    | 6:1F:150:LEU:HD22  | 2.33                     | 0.58              |
| 16:2H:119:TYR:OH   | 16:2H:131:GLU:OE1  | 2.08                     | 0.58              |
| 20:2L:172:ARG:NH2  | 47:2m:908:A:H5''   | 2.19                     | 0.58              |
| 22:2N:157:GLU:HG2  | 22:2N:159:MET:CE   | 2.33                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:2Q:91:MET:HE3  | 25:2Q:91:MET:CA    | 2.32                     | 0.58              |
| 47:2m:31:U:O2'    | 47:2m:32:U:H5'     | 2.04                     | 0.58              |
| 47:2m:183:G:H4'   | 47:2m:184:G:H5'    | 1.83                     | 0.58              |
| 47:2m:533:A:O2'   | 47:2m:534:G:OP1    | 2.20                     | 0.58              |
| 47:2m:610:G:O2'   | 47:2m:611:G:H5'    | 2.04                     | 0.58              |
| 47:2m:646:G:H2'   | 47:2m:647:U:O2     | 2.03                     | 0.58              |
| 47:2m:662:G:H4'   | 47:2m:663:C:OP1    | 2.03                     | 0.58              |
| 47:2m:1462:U:H5'' | 47:2m:1464:C:N4    | 2.18                     | 0.58              |
| 47:2m:1661:A:H8   | 67:3E:14:PHE:HB2   | 1.68                     | 0.58              |
| 53:2s:176:VAL:O   | 53:2s:180:LEU:HG   | 2.04                     | 0.58              |
| 64:3B:48:LYS:O    | 64:3B:75:ILE:HD12  | 2.03                     | 0.58              |
| 64:3B:53:GLU:HA   | 64:3B:96:GLU:OE1   | 2.03                     | 0.58              |
| 68:3F:57:ARG:HG3  | 68:3F:58:ALA:N     | 2.18                     | 0.58              |
| 74:3L:99:ALA:HB3  | 74:3L:133:THR:HG21 | 1.83                     | 0.58              |
| 1:1A:1092:G:O2'   | 1:1A:1093:C:H5'    | 2.03                     | 0.58              |
| 1:1A:1443:A:N1    | 1:1A:2102:G:N2     | 2.50                     | 0.58              |
| 1:1A:2693:G:OP1   | 39:2e:35:LYS:HE3   | 2.02                     | 0.58              |
| 1:1A:2721:G:O2'   | 1:1A:2722:G:H5'    | 2.03                     | 0.58              |
| 1:1A:3845:A:H2'   | 1:1A:3846:C:H6     | 1.68                     | 0.58              |
| 1:1A:3911:C:H2'   | 1:1A:3912:U:H6     | 1.67                     | 0.58              |
| 1:1A:5021:C:H3'   | 1:1A:5022:U:H5''   | 1.86                     | 0.58              |
| 5:1E:214:ASP:HB3  | 5:1E:363:ILE:HG23  | 1.85                     | 0.58              |
| 5:1E:300:LYS:HG3  | 5:1E:301:ASN:N     | 2.19                     | 0.58              |
| 7:1G:90:VAL:HG22  | 7:1G:91:GLY:H      | 1.69                     | 0.58              |
| 20:2L:173:ARG:O   | 20:2L:177:LEU:HG   | 2.04                     | 0.58              |
| 26:2R:122:ALA:N   | 26:2R:139:ARG:O    | 2.35                     | 0.58              |
| 43:2i:24:THR:HG22 | 43:2i:25:GLN:H     | 1.69                     | 0.58              |
| 47:2m:1415:C:H2'  | 47:2m:1417:C:C4'   | 2.32                     | 0.58              |
| 47:2m:1617:G:H4'  | 67:3E:14:PHE:CZ    | 2.39                     | 0.58              |
| 49:2o:62:LEU:HD11 | 49:2o:91:VAL:CG2   | 2.34                     | 0.58              |
| 54:2t:125:LYS:HD3 | 54:2t:128:LYS:HE2  | 1.84                     | 0.58              |
| 80:3R:103:LEU:HB3 | 80:3R:105:TYR:CD1  | 2.38                     | 0.58              |
| 1:1A:389:A:H1'    | 27:2S:90:ALA:O     | 2.03                     | 0.58              |
| 1:1A:406:C:H2'    | 1:1A:407:A:C8      | 2.38                     | 0.58              |
| 1:1A:455:C:C2'    | 1:1A:456:C:H5'     | 2.33                     | 0.58              |
| 1:1A:1200:G:C2'   | 1:1A:1201:U:H5'    | 2.32                     | 0.58              |
| 1:1A:1499:C:OP1   | 19:2K:150:ARG:NH2  | 2.36                     | 0.58              |
| 1:1A:3713:U:OP1   | 1:1A:3713:U:H4'    | 2.03                     | 0.58              |
| 1:1A:4582:C:H4'   | 5:1E:99:LEU:O      | 2.04                     | 0.58              |
| 1:1A:4911:A:OP2   | 5:1E:100:ARG:HD3   | 2.04                     | 0.58              |
| 9:2A:39:GLN:HA    | 9:2A:39:GLN:NE2    | 2.19                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:156:G:OP1   | 70:3H:2:LYS:HE3    | 2.02                     | 0.58              |
| 47:2m:338:G:H5'   | 47:2m:339:A:C8     | 2.23                     | 0.58              |
| 47:2m:787:G:N7    | 70:3H:237:LEU:HA   | 2.19                     | 0.58              |
| 47:2m:888:U:O2'   | 47:2m:889:U:H3'    | 2.04                     | 0.58              |
| 47:2m:1596:U:OP2  | 77:3O:85:ARG:NH1   | 2.37                     | 0.58              |
| 47:2m:1658:G:OP2  | 47:2m:1660:C:N4    | 2.37                     | 0.58              |
| 48:2n:141:ASN:HB2 | 63:3A:31:SER:O     | 2.04                     | 0.58              |
| 51:2q:72:ILE:HD12 | 51:2q:77:ARG:HB2   | 1.84                     | 0.58              |
| 60:2z:14:ARG:HB3  | 60:2z:14:ARG:HH11  | 1.69                     | 0.58              |
| 60:2z:21:ASP:OD2  | 60:2z:23:ARG:HD3   | 2.04                     | 0.58              |
| 66:3D:30:VAL:CG2  | 66:3D:32:VAL:HG13  | 2.33                     | 0.58              |
| 68:3F:64:HIS:HB3  | 68:3F:83:TRP:HB2   | 1.85                     | 0.58              |
| 74:3L:43:HIS:HD2  | 74:3L:55:ARG:HB2   | 1.68                     | 0.58              |
| 80:3R:113:LYS:CE  | 80:3R:115:SER:HB3  | 2.33                     | 0.58              |
| 1:1A:475:G:O2'    | 1:1A:476:G:H5'     | 2.03                     | 0.58              |
| 1:1A:1878:G:OP2   | 30:2V:14:ARG:NH1   | 2.37                     | 0.58              |
| 1:1A:2814:C:O2    | 1:1A:2814:C:H2'    | 2.03                     | 0.58              |
| 1:1A:4619:U:H2'   | 1:1A:4620:U:H6     | 1.67                     | 0.58              |
| 1:1A:4901:G:H2'   | 1:1A:4902:C:C6     | 2.39                     | 0.58              |
| 2:1B:68:C:O2'     | 2:1B:69:U:H5'      | 2.03                     | 0.58              |
| 13:2E:96:LYS:HG2  | 13:2E:163:MET:CE   | 2.31                     | 0.58              |
| 47:2m:551:U:C4    | 47:2m:552:G:O6     | 2.57                     | 0.58              |
| 47:2m:1025:U:H2'  | 47:2m:1026:C:O4'   | 2.04                     | 0.58              |
| 47:2m:1262:C:OP1  | 47:2m:1262:C:H4'   | 2.03                     | 0.58              |
| 50:2p:25:LEU:HB2  | 50:2p:34:TYR:OH    | 2.04                     | 0.58              |
| 50:2p:32:ASP:O    | 50:2p:53:THR:N     | 2.37                     | 0.58              |
| 50:2p:75:LYS:HD2  | 55:2u:22:VAL:H     | 1.69                     | 0.58              |
| 54:2t:19:LYS:NZ   | 54:2t:19:LYS:HB3   | 2.19                     | 0.58              |
| 68:3F:19:THR:HG21 | 68:3F:66:VAL:O     | 2.04                     | 0.58              |
| 69:3G:73:MET:HE1  | 69:3G:96:PHE:CZ    | 2.39                     | 0.58              |
| 69:3G:183:LYS:HG2 | 69:3G:196:ILE:HG23 | 1.86                     | 0.58              |
| 70:3H:31:ARG:O    | 70:3H:34:THR:HG23  | 2.04                     | 0.58              |
| 74:3L:72:TYR:CE2  | 74:3L:76:LEU:HD11  | 2.39                     | 0.58              |
| 76:3N:130:LYS:HB3 | 76:3N:131:PRO:HD3  | 1.86                     | 0.58              |
| 77:3O:74:SER:CA   | 77:3O:79:ILE:HB    | 2.30                     | 0.58              |
| 1:1A:76:A:H5'     | 14:2F:101:ARG:NH2  | 2.19                     | 0.58              |
| 1:1A:222:C:O2'    | 1:1A:223:G:H5'     | 2.04                     | 0.58              |
| 1:1A:318:A:H2'    | 1:1A:319:A:H8      | 1.68                     | 0.58              |
| 1:1A:1804:A:H4'   | 1:1A:1805:A:O5'    | 2.04                     | 0.58              |
| 1:1A:1907:A:H2'   | 1:1A:1908:A:C8     | 2.38                     | 0.58              |
| 1:1A:2020:U:C2'   | 1:1A:2021:G:H5''   | 2.34                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2905:C:H2'    | 1:1A:2906:G:O3'    | 2.04                     | 0.58              |
| 1:1A:3593:C:H3'    | 1:1A:3595:U:C4     | 2.39                     | 0.58              |
| 1:1A:3795:A:O2'    | 1:1A:3796:U:H5'    | 2.02                     | 0.58              |
| 1:1A:4110:C:H5'    | 1:1A:4111:U:OP2    | 2.04                     | 0.58              |
| 1:1A:4467:A:O2'    | 1:1A:4510:A:N3     | 2.33                     | 0.58              |
| 4:1D:111:THR:HB    | 4:1D:136:VAL:HG11  | 1.85                     | 0.58              |
| 11:2C:157:SER:O    | 11:2C:161:ILE:HG23 | 2.04                     | 0.58              |
| 13:2E:12:MET:HE3   | 13:2E:12:MET:CA    | 2.29                     | 0.58              |
| 28:2T:5:MET:O      | 28:2T:28:ASN:ND2   | 2.36                     | 0.58              |
| 28:2T:103:ASP:OD2  | 28:2T:106:LEU:HG   | 2.04                     | 0.58              |
| 31:2W:20:LEU:O     | 31:2W:24:SER:HB3   | 2.03                     | 0.58              |
| 47:2m:122:G:H1'    | 51:2q:144:ALA:O    | 2.03                     | 0.58              |
| 47:2m:180:G:O2'    | 47:2m:181:A:H2'    | 2.04                     | 0.58              |
| 47:2m:293:C:O2     | 47:2m:293:C:H2'    | 2.04                     | 0.58              |
| 47:2m:482:G:N1     | 47:2m:485:A:OP2    | 2.32                     | 0.58              |
| 47:2m:921:G:H3'    | 75:3M:28:ARG:HH12  | 1.69                     | 0.58              |
| 47:2m:947:G:O2'    | 47:2m:948:C:H5'    | 2.04                     | 0.58              |
| 47:2m:1016:U:H5''  | 73:3K:14:SER:HB3   | 1.85                     | 0.58              |
| 48:2n:164:ASN:O    | 48:2n:165:ASN:ND2  | 2.36                     | 0.58              |
| 49:2o:180:ASP:OD1  | 49:2o:183:GLU:HB3  | 2.04                     | 0.58              |
| 50:2p:25:LEU:CD2   | 50:2p:69:LEU:HD11  | 2.34                     | 0.58              |
| 50:2p:140:GLY:HA3  | 50:2p:182:LEU:CD1  | 2.34                     | 0.58              |
| 50:2p:211:VAL:O    | 59:2y:20:TYR:OH    | 2.19                     | 0.58              |
| 53:2s:69:LEU:HD22  | 53:2s:96:ALA:HB2   | 1.85                     | 0.58              |
| 68:3F:248:LEU:HD11 | 68:3F:259:TRP:HB2  | 1.86                     | 0.58              |
| 76:3N:10:ARG:HH12  | 76:3N:70:THR:HG23  | 1.68                     | 0.58              |
| 1:1A:1707:C:C2     | 30:2V:103:LYS:HG2  | 2.38                     | 0.57              |
| 1:1A:1766:A:C6     | 57:2w:10:ARG:HD2   | 2.38                     | 0.57              |
| 1:1A:2112:G:O2'    | 1:1A:2113:C:O5'    | 2.18                     | 0.57              |
| 1:1A:2298:U:O2'    | 1:1A:2299:G:H5'    | 2.03                     | 0.57              |
| 1:1A:4187:G:H4'    | 16:2H:82:GLY:HA2   | 1.87                     | 0.57              |
| 1:1A:4303:C:H2'    | 1:1A:4305:G:C8     | 2.39                     | 0.57              |
| 1:1A:4458:C:H2'    | 1:1A:4459:U:C6     | 2.39                     | 0.57              |
| 19:2K:177:ALA:O    | 29:2U:51:GLY:HA2   | 2.04                     | 0.57              |
| 31:2W:11:LEU:CA    | 31:2W:14:ILE:HG22  | 2.32                     | 0.57              |
| 32:2X:37:GLY:O     | 32:2X:41:ARG:HG3   | 2.04                     | 0.57              |
| 46:2l:3:SER:OG     | 46:2l:212:LYS:HA   | 2.04                     | 0.57              |
| 46:2l:113:SER:HB3  | 46:2l:116:LEU:CD2  | 2.34                     | 0.57              |
| 46:2l:117:ILE:HD11 | 46:2l:134:PHE:CZ   | 2.39                     | 0.57              |
| 47:2m:466:G:H3'    | 47:2m:466:G:N3     | 2.19                     | 0.57              |
| 47:2m:822:U:H3'    | 47:2m:824:C:OP2    | 2.04                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1238:U:O2'   | 57:2w:126:VAL:HG22 | 2.03                     | 0.57              |
| 47:2m:1283:C:H2'   | 47:2m:1286:G:O2'   | 2.04                     | 0.57              |
| 47:2m:1476:A:H1'   | 59:2y:1:MET:HE2    | 1.85                     | 0.57              |
| 50:2p:68:GLU:HB3   | 55:2u:93:THR:CG2   | 2.34                     | 0.57              |
| 56:2v:37:TYR:CE2   | 56:2v:51:ILE:HG23  | 2.39                     | 0.57              |
| 59:2y:73:LEU:HD13  | 59:2y:76:GLU:OE1   | 2.04                     | 0.57              |
| 69:3G:130:ILE:HG22 | 69:3G:158:ALA:HB1  | 1.84                     | 0.57              |
| 71:3I:111:GLN:HE22 | 71:3I:126:ALA:HB3  | 1.68                     | 0.57              |
| 76:3N:2:ASN:N      | 76:3N:32:LYS:HE2   | 2.19                     | 0.57              |
| 1:1A:2082:G:O2'    | 1:1A:2083:C:H5'    | 2.04                     | 0.57              |
| 1:1A:3756:A:H61    | 1:1A:3767:C:H42    | 1.51                     | 0.57              |
| 1:1A:4188:U:H2'    | 1:1A:4189:U:H6     | 1.69                     | 0.57              |
| 1:1A:4916:G:O2'    | 1:1A:4917:C:H5'    | 2.04                     | 0.57              |
| 1:1A:4957:C:H2'    | 1:1A:4958:C:C6     | 2.39                     | 0.57              |
| 6:1F:149:GLU:HG2   | 45:2k:72:LYS:HD3   | 1.85                     | 0.57              |
| 11:2C:12:ILE:HD12  | 11:2C:53:LYS:O     | 2.03                     | 0.57              |
| 16:2H:146:PRO:HB2  | 36:2b:104:THR:CG2  | 2.34                     | 0.57              |
| 45:2k:20:ARG:O     | 45:2k:22:LYS:N     | 2.37                     | 0.57              |
| 45:2k:47:LYS:HB3   | 45:2k:102:TYR:CZ   | 2.38                     | 0.57              |
| 46:2l:3:SER:OG     | 46:2l:213:PRO:HD3  | 2.03                     | 0.57              |
| 47:2m:188:C:H42    | 47:2m:212:C:H42    | 1.51                     | 0.57              |
| 47:2m:587:A:H5''   | 47:2m:592:C:C5     | 2.40                     | 0.57              |
| 47:2m:821:G:N2     | 71:3I:150:ARG:HG3  | 2.18                     | 0.57              |
| 47:2m:1431:G:C2    | 61:20:68:GLY:HA3   | 2.39                     | 0.57              |
| 47:2m:1481:G:H5'   | 67:3E:56:ASP:OXT   | 2.05                     | 0.57              |
| 47:2m:1677:U:OP1   | 52:2r:71:ARG:NH2   | 2.36                     | 0.57              |
| 50:2p:176:LEU:HD13 | 50:2p:181:VAL:HG12 | 1.85                     | 0.57              |
| 52:2r:38:TYR:OH    | 66:3D:54:ASP:OD2   | 2.07                     | 0.57              |
| 52:2r:50:PRO:HG2   | 52:2r:90:VAL:CG1   | 2.32                     | 0.57              |
| 54:2t:123:ARG:CZ   | 54:2t:129:LEU:HG   | 2.34                     | 0.57              |
| 60:2z:23:ARG:CB    | 77:3O:48:VAL:HG11  | 2.32                     | 0.57              |
| 68:3F:6:THR:HG23   | 68:3F:313:THR:HG21 | 1.86                     | 0.57              |
| 68:3F:131:LEU:HB2  | 68:3F:139:LYS:HZ2  | 1.69                     | 0.57              |
| 69:3G:90:GLU:HB3   | 69:3G:92:GLU:OE1   | 2.03                     | 0.57              |
| 71:3I:29:LEU:HD13  | 79:3Q:37:GLN:OE1   | 2.04                     | 0.57              |
| 72:3J:132:LYS:HE2  | 72:3J:132:LYS:HA   | 1.86                     | 0.57              |
| 73:3K:39:LYS:HA    | 73:3K:42:LYS:HE3   | 1.85                     | 0.57              |
| 1:1A:216:C:C4'     | 1:1A:219:G:H21     | 2.16                     | 0.57              |
| 1:1A:1920:C:H3'    | 1:1A:1921:C:C5'    | 2.31                     | 0.57              |
| 1:1A:1971:C:N4     | 1:1A:2001:G:O5'    | 2.37                     | 0.57              |
| 1:1A:2415:U:H2'    | 1:1A:2416:G:C8     | 2.39                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2461:G:H2'    | 1:1A:2462:C:C6     | 2.39                     | 0.57              |
| 1:1A:4210:U:O2'    | 1:1A:4211:C:H5'    | 2.04                     | 0.57              |
| 1:1A:4503:A:H2'    | 1:1A:4504:C:H6     | 1.69                     | 0.57              |
| 1:1A:4896:G:O2'    | 1:1A:4897:G:O5'    | 2.21                     | 0.57              |
| 1:1A:5027:C:OP2    | 54:2t:77:ARG:NE    | 2.36                     | 0.57              |
| 5:1E:299:ILE:HG13  | 5:1E:313:SER:HB3   | 1.86                     | 0.57              |
| 7:1G:84:PRO:HA     | 7:1G:88:VAL:O      | 2.03                     | 0.57              |
| 15:2G:132:LYS:HA   | 15:2G:135:LEU:HD22 | 1.85                     | 0.57              |
| 18:2J:116:HIS:HB3  | 18:2J:149:ILE:HB   | 1.87                     | 0.57              |
| 25:2Q:80:ARG:HD2   | 70:3H:9:ALA:O      | 2.03                     | 0.57              |
| 39:2e:13:LEU:HA    | 39:2e:16:ARG:CG    | 2.35                     | 0.57              |
| 44:2j:25:MET:HE3   | 47:2m:1040:G:H4'   | 1.85                     | 0.57              |
| 46:2l:24:LYS:HE2   | 46:2l:29:LEU:CD1   | 2.32                     | 0.57              |
| 47:2m:373:G:O2'    | 47:2m:374:G:H5'    | 2.04                     | 0.57              |
| 47:2m:399:C:N3     | 56:2v:104:LYS:HG2  | 2.19                     | 0.57              |
| 47:2m:1203:G:H4'   | 69:3G:116:THR:HA   | 1.85                     | 0.57              |
| 47:2m:1262:C:H5    | 67:3E:17:GLY:HA3   | 1.70                     | 0.57              |
| 47:2m:1419:C:C4'   | 61:20:128:GLN:HG3  | 2.34                     | 0.57              |
| 47:2m:1447:G:H2'   | 47:2m:1448:A:H8    | 1.69                     | 0.57              |
| 49:2o:60:ASP:OD1   | 49:2o:60:ASP:N     | 2.34                     | 0.57              |
| 50:2p:25:LEU:HD13  | 50:2p:50:ILE:HD12  | 1.85                     | 0.57              |
| 51:2q:21:ASP:OD1   | 51:2q:24:THR:OG1   | 2.12                     | 0.57              |
| 57:2w:127:LYS:HZ3  | 57:2w:128:HIS:HB3  | 1.69                     | 0.57              |
| 58:2x:49:TYR:HA    | 58:2x:52:LEU:CD1   | 2.35                     | 0.57              |
| 61:20:13:GLU:HA    | 61:20:16:ARG:HG2   | 1.86                     | 0.57              |
| 71:3I:110:LEU:HD23 | 71:3I:130:ILE:HD13 | 1.86                     | 0.57              |
| 77:3O:98:LYS:NZ    | 77:3O:113:THR:OG1  | 2.36                     | 0.57              |
| 1:1A:7:C:H2'       | 1:1A:8:U:H6        | 1.69                     | 0.57              |
| 1:1A:654:C:H5'     | 6:1F:268:ARG:HH22  | 1.68                     | 0.57              |
| 1:1A:742:G:H2'     | 1:1A:743:G:H8      | 1.68                     | 0.57              |
| 1:1A:1270:A:O2'    | 1:1A:1439:C:O2     | 2.23                     | 0.57              |
| 1:1A:1857:C:H2'    | 1:1A:1858:A:C8     | 2.37                     | 0.57              |
| 1:1A:2079:G:H2'    | 1:1A:2080:U:C6     | 2.39                     | 0.57              |
| 1:1A:3596:A:C3'    | 1:1A:3597:G:H5'    | 2.34                     | 0.57              |
| 1:1A:3641:U:H5     | 1:1A:3646:A:N7     | 2.02                     | 0.57              |
| 1:1A:4101:C:H2'    | 1:1A:4102:C:H5     | 1.68                     | 0.57              |
| 1:1A:4878:C:H2'    | 1:1A:4879:C:C6     | 2.38                     | 0.57              |
| 7:1G:122:GLN:HG3   | 7:1G:122:GLN:O     | 2.03                     | 0.57              |
| 23:2O:87:THR:O     | 23:2O:91:LEU:HD23  | 2.04                     | 0.57              |
| 30:2V:116:LEU:HD23 | 30:2V:116:LEU:C    | 2.29                     | 0.57              |
| 39:2e:42:LEU:HG    | 39:2e:42:LEU:O     | 2.05                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:2k:57:GLY:C     | 45:2k:58:LYS:HD3   | 2.29                     | 0.57              |
| 47:2m:168:C:O2'    | 70:3H:131:ARG:HD2  | 2.04                     | 0.57              |
| 47:2m:306:C:H2'    | 47:2m:307:G:C4     | 2.38                     | 0.57              |
| 47:2m:843:C:O2'    | 47:2m:844:U:H5'    | 2.04                     | 0.57              |
| 47:2m:1296:U:H2'   | 47:2m:1297:U:C6    | 2.40                     | 0.57              |
| 67:3E:15:GLY:O     | 67:3E:19:ARG:NH1   | 2.37                     | 0.57              |
| 68:3F:139:LYS:HG3  | 68:3F:140:TYR:HD1  | 1.69                     | 0.57              |
| 69:3G:106:VAL:HG11 | 69:3G:109:ILE:HD11 | 1.86                     | 0.57              |
| 70:3H:18:VAL:CG1   | 70:3H:24:LEU:HD21  | 2.34                     | 0.57              |
| 76:3N:38:THR:HA    | 76:3N:41:ARG:HE    | 1.70                     | 0.57              |
| 1:1A:139:G:H3'     | 1:1A:140:G:C8      | 2.39                     | 0.57              |
| 1:1A:467:U:H2'     | 1:1A:468:U:O4'     | 2.04                     | 0.57              |
| 1:1A:1558:A:H2'    | 1:1A:1559:G:H8     | 1.68                     | 0.57              |
| 1:1A:2902:G:N2     | 1:1A:3597:G:H22    | 2.02                     | 0.57              |
| 1:1A:3930:U:H2'    | 1:1A:3931:C:C6     | 2.39                     | 0.57              |
| 1:1A:4273:A:H2'    | 1:1A:4274:A:C8     | 2.40                     | 0.57              |
| 6:1F:147:VAL:O     | 45:2k:73:PRO:HG2   | 2.05                     | 0.57              |
| 7:1G:182:GLY:HA2   | 7:1G:194:VAL:CG2   | 2.33                     | 0.57              |
| 20:2L:165:LYS:O    | 20:2L:168:GLU:HG3  | 2.04                     | 0.57              |
| 25:2Q:105:ARG:HH22 | 70:3H:151:ASP:CG   | 2.12                     | 0.57              |
| 31:2W:20:LEU:CD2   | 31:2W:101:ASP:HB2  | 2.28                     | 0.57              |
| 47:2m:795:A:H3'    | 47:2m:797:C:OP2    | 2.04                     | 0.57              |
| 47:2m:996:A:H5''   | 73:3K:7:PRO:HD3    | 1.85                     | 0.57              |
| 47:2m:1819:A:O2'   | 47:2m:1820:G:H5'   | 2.04                     | 0.57              |
| 48:2n:219:GLU:HA   | 48:2n:222:VAL:HB   | 1.87                     | 0.57              |
| 49:2o:83:LYS:HD3   | 49:2o:106:THR:HG22 | 1.87                     | 0.57              |
| 51:2q:55:ALA:HA    | 51:2q:60:GLU:OE2   | 2.04                     | 0.57              |
| 52:2r:186:ASN:C    | 52:2r:191:LYS:HE2  | 2.29                     | 0.57              |
| 57:2w:127:LYS:HG3  | 57:2w:128:HIS:H    | 1.70                     | 0.57              |
| 60:2z:4:VAL:HG22   | 77:3O:55:TYR:HD2   | 1.68                     | 0.57              |
| 65:3C:58:VAL:HG13  | 74:3L:126:ILE:O    | 2.05                     | 0.57              |
| 68:3F:154:VAL:HG22 | 68:3F:167:SER:HB2  | 1.85                     | 0.57              |
| 70:3H:181:THR:O    | 70:3H:185:LEU:HG   | 2.04                     | 0.57              |
| 75:3M:108:ALA:HB3  | 75:3M:111:MET:HE1  | 1.87                     | 0.57              |
| 1:1A:483:G:N7      | 1:1A:485:C:H5''    | 2.20                     | 0.57              |
| 1:1A:1646:A:O2'    | 38:2d:49:TRP:O     | 2.21                     | 0.57              |
| 1:1A:1707:C:C5     | 30:2V:103:LYS:HE2  | 2.38                     | 0.57              |
| 1:1A:3893:C:H2'    | 1:1A:3894:A:H8     | 1.69                     | 0.57              |
| 1:1A:4486:C:C2'    | 1:1A:4487:A:H5'    | 2.34                     | 0.57              |
| 1:1A:4563:U:H2'    | 1:1A:4564:A:H8     | 1.70                     | 0.57              |
| 9:2A:91:PHE:CD2    | 9:2A:244:ILE:HD11  | 2.40                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:2F:79:GLU:O     | 14:2F:83:VAL:HG23  | 2.04                     | 0.57              |
| 37:2c:84:LYS:NZ    | 37:2c:84:LYS:HB3   | 2.20                     | 0.57              |
| 46:2l:31:THR:HG23  | 46:2l:171:HIS:HD2  | 1.70                     | 0.57              |
| 46:2l:33:GLU:OE2   | 46:2l:168:ALA:HB2  | 2.04                     | 0.57              |
| 46:2l:179:LEU:HD22 | 46:2l:183:ILE:HD11 | 1.86                     | 0.57              |
| 47:2m:549:C:H2'    | 47:2m:550:C:C5     | 2.39                     | 0.57              |
| 47:2m:933:G:H1'    | 47:2m:1001:A:O4'   | 2.05                     | 0.57              |
| 47:2m:1226:G:N1    | 47:2m:1639:G:OP2   | 2.25                     | 0.57              |
| 47:2m:1386:A:H2'   | 47:2m:1387:G:O4'   | 2.04                     | 0.57              |
| 47:2m:1628:C:H2'   | 47:2m:1629:C:C6    | 2.39                     | 0.57              |
| 53:2s:58:LYS:HE3   | 53:2s:90:LYS:HE2   | 1.86                     | 0.57              |
| 56:2v:151:THR:OG1  | 56:2v:152:LYS:N    | 2.36                     | 0.57              |
| 58:2x:38:PRO:HD3   | 61:20:8:ASP:OD1    | 2.04                     | 0.57              |
| 69:3G:152:ARG:HA   | 69:3G:155:ILE:HD12 | 1.86                     | 0.57              |
| 73:3K:34:LYS:NZ    | 73:3K:67:THR:HB    | 2.20                     | 0.57              |
| 73:3K:140:LYS:HG2  | 73:3K:142:GLU:OE2  | 2.05                     | 0.57              |
| 77:3O:56:ASP:O     | 77:3O:60:LYS:HE3   | 2.04                     | 0.57              |
| 1:1A:647:G:H2'     | 1:1A:648:G:H8      | 1.70                     | 0.57              |
| 1:1A:739:G:OP1     | 1:1A:739:G:H3'     | 2.04                     | 0.57              |
| 1:1A:1178:G:H2'    | 7:1G:286:SER:OG    | 2.05                     | 0.57              |
| 1:1A:2520:C:H2'    | 1:1A:2521:G:C8     | 2.40                     | 0.57              |
| 1:1A:3611:A:H2     | 1:1A:5016:A:H8     | 1.51                     | 0.57              |
| 5:1E:285:TYR:CG    | 5:1E:363:ILE:HD13  | 2.39                     | 0.57              |
| 13:2E:48:PRO:HB2   | 13:2E:70:VAL:CG2   | 2.34                     | 0.57              |
| 14:2F:145:LYS:HD3  | 14:2F:145:LYS:C    | 2.30                     | 0.57              |
| 14:2F:204:GLU:O    | 14:2F:207:VAL:HG12 | 2.05                     | 0.57              |
| 41:2g:78:ILE:CG2   | 41:2g:83:ARG:HH12  | 2.16                     | 0.57              |
| 46:2l:36:ILE:CD1   | 46:2l:165:LEU:HD13 | 2.30                     | 0.57              |
| 47:2m:59:U:H5''    | 47:2m:503:C:N4     | 2.20                     | 0.57              |
| 47:2m:321:C:H3'    | 47:2m:322:C:H6     | 1.69                     | 0.57              |
| 47:2m:932:G:O2'    | 47:2m:934:G:OP2    | 2.21                     | 0.57              |
| 47:2m:1025:U:OP1   | 47:2m:1090:C:O2'   | 2.22                     | 0.57              |
| 47:2m:1648:G:OP2   | 58:2x:125:ARG:HG2  | 2.04                     | 0.57              |
| 54:2t:123:ARG:HH22 | 54:2t:133:GLU:HG2  | 1.69                     | 0.57              |
| 61:20:133:ARG:HD3  | 61:20:134:ILE:N    | 2.19                     | 0.57              |
| 68:3F:8:ARG:NH2    | 68:3F:52:TYR:HA    | 2.19                     | 0.57              |
| 72:3J:64:LEU:HD11  | 80:3R:106:TYR:HD2  | 1.70                     | 0.57              |
| 1:1A:162:A:H2'     | 1:1A:163:A:H8      | 1.68                     | 0.57              |
| 1:1A:1048:G:O2'    | 1:1A:1049:C:O5'    | 2.21                     | 0.57              |
| 1:1A:1589:C:H2'    | 1:1A:1590:C:C6     | 2.40                     | 0.57              |
| 1:1A:2611:A:H4'    | 1:1A:2688:G:H4'    | 1.86                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:3893:C:H2'   | 1:1A:3894:A:C8     | 2.40                     | 0.57              |
| 1:1A:4162:C:H5    | 10:2B:73:ARG:HH12  | 1.51                     | 0.57              |
| 10:2B:138:ALA:HB1 | 10:2B:199:CYS:SG   | 2.45                     | 0.57              |
| 13:2E:93:GLU:OE1  | 13:2E:173:ILE:HG13 | 2.04                     | 0.57              |
| 14:2F:60:ARG:HD2  | 14:2F:67:HIS:O     | 2.03                     | 0.57              |
| 25:2Q:5:LEU:HA    | 25:2Q:11:TYR:O     | 2.04                     | 0.57              |
| 28:2T:73:LYS:HD3  | 28:2T:75:TYR:CZ    | 2.40                     | 0.57              |
| 31:2W:21:VAL:HG11 | 31:2W:96:ILE:CD1   | 2.35                     | 0.57              |
| 41:2g:78:ILE:HG23 | 41:2g:83:ARG:NH1   | 2.17                     | 0.57              |
| 46:2l:164:CYS:C   | 46:2l:165:LEU:HD12 | 2.29                     | 0.57              |
| 47:2m:1301:A:H4'  | 67:3E:3:HIS:NE2    | 2.20                     | 0.57              |
| 47:2m:1510:G:H2'  | 47:2m:1511:U:C6    | 2.38                     | 0.57              |
| 47:2m:1533:A:OP1  | 47:2m:1636:G:O2'   | 2.21                     | 0.57              |
| 52:2r:127:ARG:HB2 | 52:2r:136:ARG:HB3  | 1.86                     | 0.57              |
| 54:2t:142:SER:O   | 54:2t:146:GLN:HG2  | 2.04                     | 0.57              |
| 55:2u:11:ILE:HD11 | 55:2u:40:VAL:HG11  | 1.85                     | 0.57              |
| 57:2w:64:LYS:HB3  | 57:2w:65:LYS:HE2   | 1.86                     | 0.57              |
| 64:3B:82:THR:CG2  | 64:3B:118:VAL:HG22 | 2.35                     | 0.57              |
| 73:3K:4:MET:HE2   | 73:3K:124:ARG:NH1  | 2.20                     | 0.57              |
| 77:3O:87:ALA:O    | 77:3O:91:LEU:HG    | 2.05                     | 0.57              |
| 1:1A:188:G:N2     | 1:1A:189:G:O6      | 2.37                     | 0.57              |
| 1:1A:217:C:C5     | 1:1A:219:G:H4'     | 2.40                     | 0.57              |
| 1:1A:318:A:H2'    | 1:1A:319:A:C8      | 2.40                     | 0.57              |
| 1:1A:3637:U:O4    | 1:1A:3651:A:H2     | 1.87                     | 0.57              |
| 1:1A:4522:G:O2'   | 1:1A:4525:C:OP2    | 2.17                     | 0.57              |
| 1:1A:4740:G:N1    | 1:1A:4741:C:H1'    | 2.20                     | 0.57              |
| 1:1A:4741:C:H5'   | 1:1A:4742:G:OP2    | 2.05                     | 0.57              |
| 5:1E:17:LEU:HD21  | 5:1E:264:PHE:CE2   | 2.40                     | 0.57              |
| 7:1G:60:ILE:HB    | 7:1G:80:ALA:HB2    | 1.87                     | 0.57              |
| 32:2X:46:LEU:HD22 | 32:2X:72:VAL:HG11  | 1.87                     | 0.57              |
| 46:2l:60:ARG:CB   | 46:2l:61:PRO:HD3   | 2.34                     | 0.57              |
| 47:2m:333:G:H3'   | 47:2m:334:C:H5''   | 1.87                     | 0.57              |
| 47:2m:356:C:O2    | 47:2m:356:C:H2'    | 2.04                     | 0.57              |
| 47:2m:1235:G:H2'  | 47:2m:1236:G:H8    | 1.68                     | 0.57              |
| 47:2m:1276:A:N3   | 47:2m:1276:A:H2'   | 2.19                     | 0.57              |
| 47:2m:1683:C:H2'  | 47:2m:1684:C:H6    | 1.70                     | 0.57              |
| 52:2r:182:LYS:CE  | 52:2r:184:SER:HB3  | 2.34                     | 0.57              |
| 53:2s:8:ILE:HD13  | 53:2s:9:VAL:HG13   | 1.86                     | 0.57              |
| 54:2t:191:GLU:HG3 | 56:2v:19:ASN:HD22  | 1.70                     | 0.57              |
| 60:2z:84:LEU:O    | 60:2z:87:GLN:NE2   | 2.24                     | 0.57              |
| 60:2z:88:LYS:H    | 60:2z:95:TYR:HD1   | 1.53                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:21:68:THR:HG23  | 62:21:70:CYS:O     | 2.05                     | 0.57              |
| 65:3C:18:VAL:HG11  | 65:3C:33:ASP:OD2   | 2.05                     | 0.57              |
| 67:3E:21:CYS:HB3   | 67:3E:26:ASN:H     | 1.69                     | 0.57              |
| 69:3G:183:LYS:HA   | 69:3G:195:LEU:O    | 2.04                     | 0.57              |
| 70:3H:147:LEU:HD11 | 70:3H:156:TYR:HD2  | 1.70                     | 0.57              |
| 72:3J:82:ASN:OD1   | 72:3J:83:LYS:N     | 2.37                     | 0.57              |
| 73:3K:99:ARG:CZ    | 73:3K:99:ARG:HB2   | 2.33                     | 0.57              |
| 79:3Q:33:LYS:O     | 79:3Q:37:GLN:HG2   | 2.05                     | 0.57              |
| 1:1A:48:G:O2'      | 1:1A:49:U:OP2      | 2.22                     | 0.57              |
| 1:1A:2268:A:OP2    | 45:2k:11:ARG:HD2   | 2.04                     | 0.57              |
| 1:1A:2570:U:H2'    | 1:1A:2571:C:C6     | 2.40                     | 0.57              |
| 1:1A:2865:U:O2'    | 1:1A:2866:C:H5'    | 2.04                     | 0.57              |
| 1:1A:3953:G:H2'    | 1:1A:3954:A:N9     | 2.20                     | 0.57              |
| 1:1A:4063:U:H5''   | 1:1A:4064:C:H5     | 1.70                     | 0.57              |
| 1:1A:4967:A:H2'    | 1:1A:4968:A:C8     | 2.39                     | 0.57              |
| 12:2D:142:LEU:O    | 12:2D:142:LEU:HD23 | 2.05                     | 0.57              |
| 21:2M:17:LEU:HD11  | 22:2N:136:ARG:HH11 | 1.68                     | 0.57              |
| 25:2Q:101:ARG:NH1  | 25:2Q:105:ARG:HH21 | 2.01                     | 0.57              |
| 35:2a:3:GLN:HE21   | 35:2a:30:ILE:HB    | 1.70                     | 0.57              |
| 47:2m:300:U:H2'    | 47:2m:301:A:H8     | 1.69                     | 0.57              |
| 47:2m:752:G:OP2    | 47:2m:752:G:N2     | 2.38                     | 0.57              |
| 47:2m:927:C:H1'    | 78:3P:51:GLN:NE2   | 2.20                     | 0.57              |
| 53:2s:154:ILE:HG22 | 53:2s:185:VAL:HG12 | 1.87                     | 0.57              |
| 58:2x:105:LYS:O    | 58:2x:109:LYS:HG3  | 2.05                     | 0.57              |
| 66:3D:18:LEU:HB2   | 66:3D:29:GLN:HB2   | 1.86                     | 0.57              |
| 68:3F:89:LEU:HB3   | 68:3F:98:THR:OG1   | 2.05                     | 0.57              |
| 70:3H:120:ASP:HB2  | 70:3H:125:THR:HG21 | 1.86                     | 0.57              |
| 72:3J:14:VAL:HG23  | 72:3J:126:GLU:OE1  | 2.05                     | 0.57              |
| 77:3O:88:LEU:HB3   | 77:3O:109:TYR:CE2  | 2.40                     | 0.57              |
| 1:1A:83:C:OP2      | 1:1A:84:A:O2'      | 2.20                     | 0.56              |
| 1:1A:196:C:OP1     | 27:2S:122:LYS:HE2  | 2.05                     | 0.56              |
| 1:1A:307:A:O2'     | 1:1A:308:G:H5'     | 2.04                     | 0.56              |
| 1:1A:1550:G:OP1    | 20:2L:84:THR:HG21  | 2.05                     | 0.56              |
| 1:1A:1987:C:C2'    | 1:1A:1989:G:H22    | 2.17                     | 0.56              |
| 1:1A:2002:A:H2'    | 1:1A:2002:A:N3     | 2.18                     | 0.56              |
| 1:1A:2506:G:N3     | 1:1A:2506:G:H2'    | 2.20                     | 0.56              |
| 1:1A:3784:A:O2'    | 1:1A:3785:A:H3'    | 2.04                     | 0.56              |
| 1:1A:4099:G:H2'    | 1:1A:4100:C:C6     | 2.40                     | 0.56              |
| 3:1C:133:G:O2'     | 3:1C:134:G:H5'     | 2.05                     | 0.56              |
| 13:2E:54:ARG:O     | 13:2E:64:ARG:HG3   | 2.04                     | 0.56              |
| 25:2Q:96:GLN:HB2   | 25:2Q:100:VAL:CG1  | 2.33                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:2e:69:LEU:O     | 39:2e:70:LYS:HD3   | 2.05                     | 0.56              |
| 40:2f:33:ASN:O     | 40:2f:34:LYS:HG2   | 2.05                     | 0.56              |
| 47:2m:312:G:H5'    | 47:2m:313:A:OP2    | 2.05                     | 0.56              |
| 47:2m:550:C:O2'    | 47:2m:551:U:O4'    | 2.23                     | 0.56              |
| 47:2m:887:U:H5'    | 47:2m:888:U:OP2    | 2.05                     | 0.56              |
| 47:2m:1304:U:C5'   | 80:3R:95:ARG:HG2   | 2.35                     | 0.56              |
| 47:2m:1351:G:O2'   | 47:2m:1378:A:N1    | 2.35                     | 0.56              |
| 47:2m:1628:C:OP1   | 61:20:41:LYS:HB2   | 2.05                     | 0.56              |
| 47:2m:1745:A:H8    | 70:3H:65:GLN:HG3   | 1.69                     | 0.56              |
| 50:2p:25:LEU:HB2   | 50:2p:34:TYR:CZ    | 2.39                     | 0.56              |
| 52:2r:90:VAL:O     | 52:2r:93:VAL:HG12  | 2.05                     | 0.56              |
| 60:2z:5:ILE:HD13   | 77:3O:49:LEU:CB    | 2.31                     | 0.56              |
| 68:3F:83:TRP:CA    | 68:3F:107:ASP:HB2  | 2.30                     | 0.56              |
| 73:3K:5:HIS:CD2    | 73:3K:121:ARG:HG3  | 2.40                     | 0.56              |
| 1:1A:7:C:O2'       | 1:1A:8:U:H5'       | 2.05                     | 0.56              |
| 1:1A:647:G:H2'     | 1:1A:648:G:C8      | 2.39                     | 0.56              |
| 1:1A:652:G:H2'     | 1:1A:653:U:H6      | 1.70                     | 0.56              |
| 1:1A:1340:C:O2'    | 1:1A:1341:U:H5'    | 2.05                     | 0.56              |
| 1:1A:1749:A:H2'    | 1:1A:1750:G:H8     | 1.70                     | 0.56              |
| 1:1A:2483:G:H3'    | 1:1A:2484:A:H5''   | 1.85                     | 0.56              |
| 1:1A:2824:C:O2'    | 1:1A:2825:A:H5'    | 2.05                     | 0.56              |
| 1:1A:4599:A:H4'    | 1:1A:4600:G:OP1    | 2.04                     | 0.56              |
| 1:1A:4992:G:O2'    | 1:1A:4993:G:H5'    | 2.05                     | 0.56              |
| 1:1A:5061:A:H4'    | 1:1A:5062:G:C5'    | 2.35                     | 0.56              |
| 4:1D:24:LYS:HG3    | 4:1D:49:ILE:HD12   | 1.84                     | 0.56              |
| 17:2L:54:TYR:HD1   | 17:2L:145:VAL:HG21 | 1.70                     | 0.56              |
| 20:2L:7:GLN:OE1    | 20:2L:7:GLN:N      | 2.37                     | 0.56              |
| 47:2m:50:A:H2'     | 47:2m:51:U:H5'     | 1.87                     | 0.56              |
| 47:2m:65:C:O3'     | 70:3H:172:LYS:HE3  | 2.05                     | 0.56              |
| 47:2m:751:G:N2     | 47:2m:752:G:H1'    | 2.19                     | 0.56              |
| 47:2m:794:A:H2'    | 47:2m:795:A:C4'    | 2.29                     | 0.56              |
| 47:2m:1542:C:O2'   | 47:2m:1543:U:O5'   | 2.20                     | 0.56              |
| 47:2m:1562:C:H4'   | 61:20:119:GLY:HA3  | 1.86                     | 0.56              |
| 47:2m:1613:G:OP1   | 57:2w:42:ARG:NH2   | 2.37                     | 0.56              |
| 49:2o:168:MET:HG2  | 49:2o:197:ILE:CG2  | 2.34                     | 0.56              |
| 50:2p:68:GLU:HB3   | 55:2u:93:THR:HG21  | 1.87                     | 0.56              |
| 50:2p:176:LEU:HD12 | 50:2p:180:GLY:O    | 2.05                     | 0.56              |
| 54:2t:139:LYS:HB2  | 54:2t:141:ARG:CD   | 2.33                     | 0.56              |
| 69:3G:183:LYS:HE2  | 75:3M:95:PRO:HA    | 1.86                     | 0.56              |
| 70:3H:64:LYS:CE    | 70:3H:82:SER:HB3   | 2.34                     | 0.56              |
| 76:3N:16:ARG:H     | 76:3N:16:ARG:CD    | 2.17                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 77:3O:96:LEU:HD23 | 77:3O:96:LEU:H    | 1.70                     | 0.56              |
| 1:1A:31:U:H2'     | 1:1A:32:G:O4'     | 2.05                     | 0.56              |
| 1:1A:65:A:N6      | 1:1A:75:G:H1'     | 2.20                     | 0.56              |
| 1:1A:106:A:O4'    | 1:1A:336:A:H1'    | 2.05                     | 0.56              |
| 1:1A:1707:C:H2'   | 30:2V:103:LYS:HG3 | 1.87                     | 0.56              |
| 1:1A:2080:U:O2'   | 1:1A:2081:C:H5'   | 2.05                     | 0.56              |
| 1:1A:2553:A:H2    | 1:1A:2764:A:H62   | 1.51                     | 0.56              |
| 1:1A:2725:A:H3'   | 1:1A:2725:A:OP1   | 2.06                     | 0.56              |
| 1:1A:4253:A:H5'   | 1:1A:4254:G:C8    | 2.41                     | 0.56              |
| 1:1A:4291:G:OP2   | 43:2i:10:THR:HG22 | 2.05                     | 0.56              |
| 1:1A:4503:A:H2'   | 1:1A:4504:C:C6    | 2.41                     | 0.56              |
| 1:1A:4903:G:O2'   | 1:1A:4904:G:H5'   | 2.04                     | 0.56              |
| 1:1A:5024:C:H42   | 1:1A:5029:C:C4'   | 2.19                     | 0.56              |
| 3:1C:62:A:OP1     | 36:2b:51:ARG:NH2  | 2.34                     | 0.56              |
| 3:1C:67:U:H2'     | 3:1C:68:G:C8      | 2.40                     | 0.56              |
| 5:1E:308:ASP:OD1  | 5:1E:309:LEU:N    | 2.38                     | 0.56              |
| 7:1G:238:GLU:OE1  | 7:1G:238:GLU:HA   | 2.05                     | 0.56              |
| 8:1H:176:THR:HB   | 8:1H:186:LEU:HD23 | 1.87                     | 0.56              |
| 8:1H:222:LEU:H    | 8:1H:237:LYS:HE3  | 1.69                     | 0.56              |
| 14:2F:145:LYS:HG3 | 14:2F:146:LEU:CD1 | 2.34                     | 0.56              |
| 17:2I:110:PRO:N   | 17:2I:111:PRO:HD2 | 2.19                     | 0.56              |
| 18:2J:15:CYS:SG   | 18:2J:102:ALA:HB2 | 2.44                     | 0.56              |
| 31:2W:38:ILE:HG21 | 31:2W:63:TYR:HB3  | 1.87                     | 0.56              |
| 36:2b:89:ARG:O    | 36:2b:93:ARG:HG2  | 2.05                     | 0.56              |
| 46:2l:67:VAL:HG12 | 46:2l:111:LEU:CB  | 2.33                     | 0.56              |
| 47:2m:329:G:H2'   | 47:2m:330:G:C1'   | 2.35                     | 0.56              |
| 47:2m:896:U:H4'   | 47:2m:897:U:OP1   | 2.03                     | 0.56              |
| 47:2m:927:C:H1'   | 78:3P:51:GLN:HE22 | 1.70                     | 0.56              |
| 47:2m:945:U:H2'   | 47:2m:946:U:H6    | 1.67                     | 0.56              |
| 47:2m:958:G:O2'   | 47:2m:959:G:H5'   | 2.05                     | 0.56              |
| 47:2m:1337:C:H4'  | 62:21:67:LYS:O    | 2.05                     | 0.56              |
| 47:2m:1339:U:O2'  | 47:2m:1340:U:H5'  | 2.05                     | 0.56              |
| 47:2m:1491:G:H2'  | 47:2m:1492:U:C6   | 2.40                     | 0.56              |
| 47:2m:1754:G:H3'  | 47:2m:1755:C:C5'  | 2.35                     | 0.56              |
| 48:2n:190:SER:H   | 48:2n:193:HIS:HE1 | 1.52                     | 0.56              |
| 49:2o:62:LEU:HD11 | 49:2o:91:VAL:HG21 | 1.86                     | 0.56              |
| 49:2o:196:ASP:HA  | 49:2o:199:LYS:HE3 | 1.86                     | 0.56              |
| 49:2o:226:GLY:O   | 49:2o:230:GLU:HG3 | 2.05                     | 0.56              |
| 50:2p:72:VAL:CG1  | 55:2u:20:VAL:HB   | 2.36                     | 0.56              |
| 50:2p:150:MET:SD  | 50:2p:150:MET:N   | 2.78                     | 0.56              |
| 53:2s:101:LEU:HB2 | 53:2s:120:ARG:HB3 | 1.86                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:2t:123:ARG:HD2 | 54:2t:129:LEU:CD2  | 2.35                     | 0.56              |
| 57:2w:18:ARG:HH12 | 60:2z:90:VAL:HG22  | 1.70                     | 0.56              |
| 58:2x:29:ASN:N    | 58:2x:67:ASP:OD1   | 2.39                     | 0.56              |
| 59:2y:99:ASP:OD1  | 59:2y:102:THR:HG22 | 2.05                     | 0.56              |
| 60:2z:64:VAL:O    | 60:2z:68:ILE:HG12  | 2.05                     | 0.56              |
| 62:21:48:LEU:O    | 62:21:50:VAL:HG23  | 2.06                     | 0.56              |
| 65:3C:45:VAL:HG21 | 65:3C:64:LEU:CG    | 2.34                     | 0.56              |
| 68:3F:101:PHE:HB3 | 68:3F:132:TRP:CZ3  | 2.40                     | 0.56              |
| 69:3G:59:GLU:OE1  | 69:3G:59:GLU:N     | 2.38                     | 0.56              |
| 70:3H:49:VAL:HG21 | 70:3H:115:LYS:HE3  | 1.87                     | 0.56              |
| 71:3I:111:GLN:OE1 | 71:3I:127:ARG:HA   | 2.06                     | 0.56              |
| 72:3J:48:HIS:CB   | 72:3J:111:VAL:HG23 | 2.34                     | 0.56              |
| 1:1A:36:U:OP1     | 1:1A:1651:G:N2     | 2.38                     | 0.56              |
| 1:1A:1079:C:H2'   | 1:1A:1080:C:N1     | 2.19                     | 0.56              |
| 1:1A:1528:U:H2'   | 1:1A:1529:G:C8     | 2.41                     | 0.56              |
| 1:1A:2403:A:OP1   | 35:2a:10:ARG:HD3   | 2.05                     | 0.56              |
| 1:1A:3909:C:O2    | 1:1A:3909:C:H2'    | 2.05                     | 0.56              |
| 1:1A:4538:G:H2'   | 1:1A:4539:U:C6     | 2.40                     | 0.56              |
| 4:1D:111:THR:HB   | 4:1D:136:VAL:CG1   | 2.35                     | 0.56              |
| 11:2C:92:MET:HE2  | 11:2C:161:ILE:HD11 | 1.87                     | 0.56              |
| 17:2I:186:GLU:OE2 | 17:2I:187:LYS:HG2  | 2.04                     | 0.56              |
| 47:2m:115:U:H2'   | 47:2m:116:U:C6     | 2.41                     | 0.56              |
| 47:2m:428:U:O4'   | 71:3I:2:PRO:HG2    | 2.04                     | 0.56              |
| 47:2m:496:C:OP1   | 51:2q:49:ARG:NH2   | 2.38                     | 0.56              |
| 47:2m:562:U:H2'   | 47:2m:563:G:C8     | 2.40                     | 0.56              |
| 47:2m:1538:C:H2'  | 47:2m:1539:U:H6    | 1.69                     | 0.56              |
| 48:2n:68:ILE:HG23 | 48:2n:120:ARG:NH2  | 2.21                     | 0.56              |
| 51:2q:26:VAL:HG21 | 71:3I:2:PRO:O      | 2.05                     | 0.56              |
| 51:2q:104:ASP:O   | 51:2q:190:GLY:HA3  | 2.05                     | 0.56              |
| 53:2s:75:ILE:HG13 | 53:2s:79:LEU:HD12  | 1.87                     | 0.56              |
| 59:2y:66:VAL:HG13 | 59:2y:66:VAL:O     | 2.06                     | 0.56              |
| 59:2y:71:ILE:HD12 | 59:2y:71:ILE:N     | 2.21                     | 0.56              |
| 59:2y:99:ASP:OD1  | 59:2y:101:ASP:HB2  | 2.05                     | 0.56              |
| 62:21:24:LEU:CD1  | 62:21:32:LEU:HD11  | 2.35                     | 0.56              |
| 68:3F:19:THR:N    | 68:3F:34:ALA:O     | 2.31                     | 0.56              |
| 68:3F:22:ALA:HB3  | 68:3F:32:LEU:HG    | 1.88                     | 0.56              |
| 70:3H:147:LEU:HB3 | 70:3H:151:ASP:CB   | 2.35                     | 0.56              |
| 73:3K:34:LYS:HZ3  | 73:3K:67:THR:HB    | 1.70                     | 0.56              |
| 77:3O:56:ASP:HB3  | 77:3O:60:LYS:NZ    | 2.21                     | 0.56              |
| 1:1A:84:A:H4'     | 1:1A:85:G:OP1      | 2.05                     | 0.56              |
| 1:1A:512:U:H2'    | 1:1A:513:U:H5'     | 1.88                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1174:G:H1    | 1:1A:1186:U:H3     | 1.51                     | 0.56              |
| 1:1A:1241:C:O2    | 1:1A:1241:C:H3'    | 2.06                     | 0.56              |
| 1:1A:1755:C:O2'   | 1:1A:1756:U:H5'    | 2.06                     | 0.56              |
| 1:1A:2674:A:H4'   | 1:1A:2675:G:OP2    | 2.06                     | 0.56              |
| 1:1A:2894:A:O2'   | 1:1A:2895:A:H5'    | 2.05                     | 0.56              |
| 1:1A:2899:C:OP1   | 20:2L:108:ARG:NH2  | 2.39                     | 0.56              |
| 1:1A:4688:C:H2'   | 1:1A:4689:U:C6     | 2.41                     | 0.56              |
| 1:1A:4929:C:O2'   | 1:1A:4930:C:H5'    | 2.05                     | 0.56              |
| 10:2B:120:LYS:O   | 10:2B:125:LYS:HG2  | 2.06                     | 0.56              |
| 10:2B:162:ASP:CB  | 10:2B:163:PRO:HD3  | 2.29                     | 0.56              |
| 11:2C:174:LYS:HG2 | 11:2C:175:PHE:H    | 1.70                     | 0.56              |
| 47:2m:303:C:O2'   | 47:2m:304:C:OP1    | 2.16                     | 0.56              |
| 47:2m:558:G:H2'   | 47:2m:559:G:C2     | 2.40                     | 0.56              |
| 47:2m:1409:A:C5'  | 58:2x:26:LYS:HD3   | 2.35                     | 0.56              |
| 47:2m:1420:G:OP2  | 61:20:129:ARG:HG3  | 2.05                     | 0.56              |
| 47:2m:1505:U:H1'  | 47:2m:1508:A:C2    | 2.41                     | 0.56              |
| 47:2m:1521:C:OP2  | 60:2z:136:THR:OG1  | 2.10                     | 0.56              |
| 48:2n:12:GLU:N    | 48:2n:12:GLU:OE1   | 2.39                     | 0.56              |
| 48:2n:38:ILE:HD11 | 48:2n:150:THR:HG22 | 1.87                     | 0.56              |
| 48:2n:57:LYS:NZ   | 48:2n:160:ALA:O    | 2.28                     | 0.56              |
| 49:2o:185:VAL:O   | 49:2o:189:ILE:HG13 | 2.04                     | 0.56              |
| 50:2p:76:ARG:HH21 | 50:2p:77:PHE:HA    | 1.69                     | 0.56              |
| 52:2r:110:GLN:O   | 52:2r:113:VAL:HG22 | 2.04                     | 0.56              |
| 54:2t:172:LEU:CD1 | 54:2t:190:LEU:HB2  | 2.35                     | 0.56              |
| 56:2v:150:GLY:HA2 | 56:2v:153:LYS:NZ   | 2.19                     | 0.56              |
| 59:2y:21:TYR:CE1  | 59:2y:71:ILE:HD13  | 2.40                     | 0.56              |
| 60:2z:30:ILE:O    | 60:2z:33:ILE:HG22  | 2.06                     | 0.56              |
| 61:20:133:ARG:O   | 61:20:137:GLN:HG2  | 2.05                     | 0.56              |
| 67:3E:2:GLY:HA3   | 67:3E:6:LEU:CD1    | 2.31                     | 0.56              |
| 71:3I:101:LYS:HG2 | 71:3I:103:GLU:OE1  | 2.05                     | 0.56              |
| 77:3O:89:GLN:O    | 77:3O:92:LEU:HB2   | 2.05                     | 0.56              |
| 1:1A:324:A:H2'    | 1:1A:325:U:C6      | 2.41                     | 0.56              |
| 1:1A:1366:G:C3'   | 1:1A:1367:C:H5''   | 2.36                     | 0.56              |
| 1:1A:3880:G:H2'   | 1:1A:3881:G:C8     | 2.40                     | 0.56              |
| 1:1A:4980:C:N3    | 18:2J:69:ARG:NH2   | 2.50                     | 0.56              |
| 1:1A:5024:C:H41   | 1:1A:5028:G:H2'    | 1.69                     | 0.56              |
| 8:1H:237:LYS:O    | 8:1H:237:LYS:HD3   | 2.05                     | 0.56              |
| 18:2J:125:MET:HB2 | 18:2J:141:SER:OG   | 2.06                     | 0.56              |
| 25:2Q:96:GLN:CB   | 25:2Q:100:VAL:HG11 | 2.35                     | 0.56              |
| 46:2L:120:ILE:CG2 | 46:2L:124:LEU:HD13 | 2.32                     | 0.56              |
| 47:2m:524:U:H5''  | 47:2m:525:A:O4'    | 2.06                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:912:C:H2'    | 47:2m:912:C:OP2    | 2.05                     | 0.56              |
| 47:2m:1460:C:N4    | 47:2m:1461:G:O6    | 2.39                     | 0.56              |
| 47:2m:1693:G:N2    | 47:2m:1834:A:H8    | 2.03                     | 0.56              |
| 47:2m:1802:C:OP2   | 81:2m:1901:84D:N   | 2.39                     | 0.56              |
| 51:2q:192:ILE:HD12 | 51:2q:243:GLY:HA3  | 1.87                     | 0.56              |
| 52:2r:40:ALA:CB    | 52:2r:67:PRO:HA    | 2.36                     | 0.56              |
| 52:2r:62:ARG:HG3   | 52:2r:62:ARG:O     | 2.05                     | 0.56              |
| 53:2s:160:LYS:HG2  | 53:2s:160:LYS:O    | 2.06                     | 0.56              |
| 55:2u:1:MET:HE2    | 55:2u:47:LYS:HB3   | 1.87                     | 0.56              |
| 59:2y:53:TYR:O     | 59:2y:57:LEU:HD23  | 2.05                     | 0.56              |
| 61:20:115:LYS:HA   | 61:20:121:ARG:HA   | 1.87                     | 0.56              |
| 62:21:38:ASP:OD1   | 62:21:41:ARG:NE    | 2.32                     | 0.56              |
| 70:3H:190:ARG:O    | 70:3H:194:LEU:HG   | 2.05                     | 0.56              |
| 77:3O:58:LEU:O     | 77:3O:63:PRO:HD3   | 2.06                     | 0.56              |
| 1:1A:1415:G:O2'    | 1:1A:1416:G:H5'    | 2.06                     | 0.56              |
| 1:1A:1783:C:C2'    | 1:1A:1784:U:H5'    | 2.36                     | 0.56              |
| 1:1A:2464:C:O2'    | 1:1A:2465:C:H6     | 1.88                     | 0.56              |
| 1:1A:3633:C:H2'    | 1:1A:3634:G:H8     | 1.70                     | 0.56              |
| 3:1C:84:A:N3       | 3:1C:84:A:H2'      | 2.21                     | 0.56              |
| 10:2B:187:LYS:HG3  | 10:2B:198:THR:HB   | 1.87                     | 0.56              |
| 11:2C:116:ASN:OD1  | 11:2C:119:GLY:HA2  | 2.05                     | 0.56              |
| 13:2E:118:LYS:HD2  | 13:2E:118:LYS:C    | 2.30                     | 0.56              |
| 14:2F:87:HIS:HB3   | 14:2F:90:VAL:HG13  | 1.87                     | 0.56              |
| 46:2I:96:ASN:HD21  | 46:2I:125:GLY:HA3  | 1.70                     | 0.56              |
| 46:2I:106:LYS:HD2  | 46:2I:107:TYR:CB   | 2.35                     | 0.56              |
| 47:2m:1097:G:O2'   | 47:2m:1098:C:H5'   | 2.05                     | 0.56              |
| 47:2m:1435:C:H5''  | 47:2m:1436:C:O4'   | 2.05                     | 0.56              |
| 55:2u:90:VAL:HB    | 55:2u:94:LEU:CG    | 2.32                     | 0.56              |
| 58:2x:89:SER:O     | 58:2x:92:LEU:HG    | 2.06                     | 0.56              |
| 68:3F:44:LYS:HD3   | 68:3F:45:LEU:H     | 1.70                     | 0.56              |
| 70:3H:181:THR:HG23 | 70:3H:183:ARG:H    | 1.70                     | 0.56              |
| 71:3I:136:ARG:HG2  | 71:3I:159:PHE:C    | 2.30                     | 0.56              |
| 77:3O:100:VAL:HB   | 77:3O:108:ILE:HG22 | 1.88                     | 0.56              |
| 1:1A:467:U:N3      | 1:1A:468:U:H1'     | 2.21                     | 0.56              |
| 1:1A:721:G:O2'     | 1:1A:722:G:H5'     | 2.06                     | 0.56              |
| 1:1A:1079:C:H2'    | 1:1A:1080:C:C1'    | 2.35                     | 0.56              |
| 1:1A:1431:C:O2'    | 1:1A:1432:G:H5'    | 2.04                     | 0.56              |
| 1:1A:1875:C:H2'    | 1:1A:1876:U:C6     | 2.40                     | 0.56              |
| 1:1A:1961:G:H2'    | 1:1A:2024:G:N2     | 2.21                     | 0.56              |
| 1:1A:2267:U:OP1    | 45:2k:37:SER:HB2   | 2.05                     | 0.56              |
| 1:1A:2483:G:H2'    | 1:1A:2484:A:O4'    | 2.06                     | 0.56              |

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| Atom-1             | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------------|--------------------------|-------------------|
| 1:1A:2557:G:H1     | 1:1A:2570:U:H3        | 1.53                     | 0.56              |
| 1:1A:2639:U:H2'    | 1:1A:2694:G:H1        | 1.70                     | 0.56              |
| 1:1A:2694:G:H4'    | 1:1A:2695:A:C5'       | 2.31                     | 0.56              |
| 1:1A:4088:C:H2'    | 1:1A:4089:G:C8        | 2.40                     | 0.56              |
| 1:1A:4966:A:H5'    | 5:1E:128:LYS:HG3      | 1.87                     | 0.56              |
| 3:1C:44:A:O2'      | 3:1C:45:C:H5'         | 2.06                     | 0.56              |
| 13:2E:31:ASP:CA    | 13:2E:34:THR:HG22     | 2.35                     | 0.56              |
| 16:2H:84:PRO:HA    | 16:2H:87:HIS:CG       | 2.41                     | 0.56              |
| 23:2O:27:HIS:HB3   | 23:2O:114:TYR:HE1     | 1.70                     | 0.56              |
| 33:2Y:35:TRP:CZ2   | 33:2Y:56:PRO:HD2      | 2.41                     | 0.56              |
| 33:2Y:127:ALA:O    | 33:2Y:128:ARG:HD3     | 2.06                     | 0.56              |
| 46:2L:12:GLU:HG3   | 46:2L:216:LEU:HA      | 1.88                     | 0.56              |
| 47:2m:1554:C:H5''  | 47:2m:1555:U:H1'      | 1.85                     | 0.56              |
| 49:2o:34:LYS:NZ    | 49:2o:43:ASN:HB2      | 2.20                     | 0.56              |
| 50:2p:132:LYS:HD3  | 50:2p:156:LEU:HD23    | 1.87                     | 0.56              |
| 52:2r:127:ARG:HH12 | 52:2r:128:ILE:HG13    | 1.70                     | 0.56              |
| 55:2u:55:ARG:NH1   | 55:2u:78:TYR:OH       | 2.39                     | 0.56              |
| 62:21:40:ILE:HD11  | 62:21:53:PRO:HG3      | 1.88                     | 0.56              |
| 62:21:61:LEU:HD23  | 67:3E:34:TYR:CE2      | 2.41                     | 0.56              |
| 64:3B:125:VAL:O    | 64:3B:128:VAL:HG12    | 2.06                     | 0.56              |
| 66:3D:13:ARG:HB3   | 66:3D:33:GLU:OE2      | 2.06                     | 0.56              |
| 68:3F:32:LEU:CD2   | 68:3F:71:ILE:HD11     | 2.14                     | 0.56              |
| 68:3F:41:ILE:HG22  | 68:3F:43:TRP:CD1      | 2.40                     | 0.56              |
| 68:3F:191:HIS:CD2  | 68:3F:217:MET:HE3     | 2.41                     | 0.56              |
| 76:3N:109:GLU:HG3  | 76:3N:113[A]:ARG:HH22 | 1.71                     | 0.56              |
| 1:1A:72:C:O4'      | 37:2c:15:HIS:HB3      | 2.06                     | 0.56              |
| 1:1A:386:A:H3'     | 1:1A:387:G:H5''       | 1.88                     | 0.56              |
| 1:1A:907:C:H2'     | 1:1A:908:G:C8         | 2.41                     | 0.56              |
| 1:1A:978:G:H2'     | 1:1A:979:C:H6         | 1.69                     | 0.56              |
| 1:1A:1320:U:O2'    | 1:1A:1891:A:N1        | 2.35                     | 0.56              |
| 1:1A:1418:C:H2'    | 1:1A:1419:G:O4'       | 2.06                     | 0.56              |
| 1:1A:1423:U:O2'    | 1:1A:1424:G:H5'       | 2.05                     | 0.56              |
| 1:1A:1443:A:H2'    | 1:1A:1444:G:C1'       | 2.36                     | 0.56              |
| 1:1A:1821:G:H2'    | 1:1A:1821:G:N3        | 2.20                     | 0.56              |
| 1:1A:2314:G:O2'    | 1:1A:2315:G:H5'       | 2.06                     | 0.56              |
| 1:1A:2809:G:O2'    | 1:1A:4644:G:OP1       | 2.23                     | 0.56              |
| 1:1A:3976:C:H2'    | 1:1A:3977:C:C6        | 2.41                     | 0.56              |
| 1:1A:4457:U:H1'    | 5:1E:252:ALA:HB3      | 1.87                     | 0.56              |
| 1:1A:4989:U:O2'    | 1:1A:4991:U:H4'       | 2.06                     | 0.56              |
| 9:2A:60:GLU:O      | 9:2A:64:MET:HG2       | 2.06                     | 0.56              |
| 12:2D:101:LYS:NZ   | 12:2D:112:GLN:HG2     | 2.20                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:2F:63:THR:HG21  | 29:2U:66:ASN:HB3  | 1.88                     | 0.56              |
| 31:2W:11:LEU:O     | 31:2W:14:ILE:HG22 | 2.06                     | 0.56              |
| 43:2i:56:PHE:O     | 43:2i:57:ARG:HG2  | 2.06                     | 0.56              |
| 47:2m:550:C:H2'    | 47:2m:551:U:C6    | 2.40                     | 0.56              |
| 47:2m:1545:A:C3'   | 58:2x:74:GLY:HA2  | 2.36                     | 0.56              |
| 47:2m:1550:G:H5'   | 47:2m:1551:U:OP1  | 2.06                     | 0.56              |
| 47:2m:1849:G:O2'   | 47:2m:1850:A:H8   | 1.88                     | 0.56              |
| 57:2w:34:MET:HE3   | 57:2w:45:LEU:HB2  | 1.86                     | 0.56              |
| 61:20:39:LEU:HD13  | 61:20:47:PRO:HG3  | 1.88                     | 0.56              |
| 62:21:29:VAL:HG23  | 62:21:85:HIS:CD2  | 2.41                     | 0.56              |
| 66:3D:14:VAL:HG23  | 66:3D:32:VAL:CG1  | 2.36                     | 0.56              |
| 68:3F:17:TRP:HD1   | 68:3F:303:THR:HA  | 1.70                     | 0.56              |
| 71:3I:82:VAL:HG21  | 71:3I:92:MET:HE2  | 1.86                     | 0.56              |
| 80:3R:121:CYS:HA   | 80:3R:132:MET:CE  | 2.31                     | 0.56              |
| 1:1A:192:G:O2'     | 1:1A:193:G:H5'    | 2.06                     | 0.56              |
| 1:1A:493:G:N1      | 1:1A:661:C:O2     | 2.35                     | 0.56              |
| 1:1A:2495:U:H2'    | 1:1A:2496:G:N7    | 2.20                     | 0.56              |
| 1:1A:2850:A:O3'    | 1:1A:4495:G:H5'   | 2.06                     | 0.56              |
| 1:1A:4934:A:H2'    | 1:1A:4935:C:C6    | 2.41                     | 0.56              |
| 1:1A:4968:A:H2'    | 1:1A:4969:C:H6    | 1.71                     | 0.56              |
| 1:1A:5001:U:H2'    | 1:1A:5002:U:O4'   | 2.06                     | 0.56              |
| 2:1B:33:U:H2'      | 2:1B:34:C:C6      | 2.41                     | 0.56              |
| 6:1F:211:TYR:OH    | 6:1F:218:ILE:HD11 | 2.06                     | 0.56              |
| 8:1H:221:LYS:HA    | 8:1H:237:LYS:NZ   | 2.21                     | 0.56              |
| 11:2C:128:MET:HE2  | 11:2C:128:MET:HA  | 1.88                     | 0.56              |
| 47:2m:327:G:H1'    | 47:2m:328:U:C1'   | 2.36                     | 0.56              |
| 47:2m:398:A:C4'    | 47:2m:399:C:H5''  | 2.36                     | 0.56              |
| 47:2m:428:U:C4'    | 71:3I:2:PRO:HG2   | 2.36                     | 0.56              |
| 50:2p:70:THR:CG2   | 50:2p:86:LEU:HD12 | 2.36                     | 0.56              |
| 52:2r:44:LYS:O     | 52:2r:44:LYS:HD3  | 2.06                     | 0.56              |
| 52:2r:142:SER:HA   | 66:3D:56:LEU:HD23 | 1.87                     | 0.56              |
| 52:2r:182:LYS:HG3  | 52:2r:183:GLY:N   | 2.20                     | 0.56              |
| 53:2s:134:VAL:HG12 | 53:2s:173:PHE:CE2 | 2.41                     | 0.56              |
| 56:2v:37:TYR:CD2   | 56:2v:51:ILE:HG12 | 2.40                     | 0.56              |
| 57:2w:25:LEU:HD11  | 57:2w:87:PRO:CG   | 2.36                     | 0.56              |
| 59:2y:73:LEU:O     | 59:2y:76:GLU:HG2  | 2.06                     | 0.56              |
| 60:2z:51:ASP:N     | 60:2z:51:ASP:OD1  | 2.37                     | 0.56              |
| 68:3F:131:LEU:HB2  | 68:3F:139:LYS:NZ  | 2.21                     | 0.56              |
| 79:3Q:8:ARG:O      | 79:3Q:8:ARG:CG    | 2.54                     | 0.56              |
| 1:1A:1774:C:H2'    | 1:1A:1775:A:O4'   | 2.05                     | 0.55              |
| 1:1A:4507:A:H2'    | 1:1A:4508:C:C6    | 2.41                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4750:G:H22   | 34:2Z:52:LYS:CE    | 2.18                     | 0.55              |
| 1:1A:4880:C:C2'   | 1:1A:4881:U:H5'    | 2.35                     | 0.55              |
| 4:1D:142:GLU:O    | 4:1D:143:THR:OG1   | 2.21                     | 0.55              |
| 6:1F:144:ILE:HD13 | 6:1F:150:LEU:HD13  | 1.89                     | 0.55              |
| 26:2R:80:PRO:HG2  | 26:2R:155:ILE:CG2  | 2.34                     | 0.55              |
| 30:2V:117:ARG:HG3 | 30:2V:117:ARG:O    | 2.06                     | 0.55              |
| 32:2X:68:LEU:HD22 | 32:2X:106:VAL:O    | 2.06                     | 0.55              |
| 47:2m:176:U:H2'   | 47:2m:177:G:O4'    | 2.05                     | 0.55              |
| 47:2m:579:C:HO2'  | 47:2m:580:U:P      | 2.29                     | 0.55              |
| 47:2m:612:U:H2'   | 47:2m:612:U:O2     | 2.04                     | 0.55              |
| 47:2m:1745:A:C8   | 70:3H:65:GLN:HG3   | 2.41                     | 0.55              |
| 47:2m:1778:C:H2'  | 47:2m:1779:G:H8    | 1.70                     | 0.55              |
| 47:2m:1809:A:O2'  | 47:2m:1810:U:H5'   | 2.06                     | 0.55              |
| 47:2m:1855:G:OP2  | 74:3L:147:ARG:NH2  | 2.39                     | 0.55              |
| 53:2s:18:GLU:O    | 53:2s:20:GLU:HG2   | 2.06                     | 0.55              |
| 53:2s:144:ILE:H   | 53:2s:144:ILE:CD1  | 2.19                     | 0.55              |
| 56:2v:7:GLU:HG3   | 56:2v:11:GLN:NE2   | 2.21                     | 0.55              |
| 57:2w:18:ARG:NE   | 57:2w:36:LEU:O     | 2.35                     | 0.55              |
| 68:3F:52:TYR:CE2  | 68:3F:309:VAL:HG11 | 2.41                     | 0.55              |
| 71:3I:94:LEU:HA   | 71:3I:97:ILE:CD1   | 2.36                     | 0.55              |
| 77:3O:54:THR:HA   | 77:3O:57:LYS:HD3   | 1.88                     | 0.55              |
| 1:1A:461:G:O2'    | 1:1A:462:G:H5'     | 2.06                     | 0.55              |
| 1:1A:492:U:OP1    | 6:1F:1:MET:HE1     | 2.06                     | 0.55              |
| 1:1A:3598:C:H2'   | 1:1A:3599:A:H8     | 1.71                     | 0.55              |
| 1:1A:4473:A:O2'   | 1:1A:4474:A:H5'    | 2.05                     | 0.55              |
| 1:1A:4576:U:H2'   | 1:1A:4577:U:C6     | 2.41                     | 0.55              |
| 21:2M:164:LYS:HA  | 21:2M:164:LYS:CE   | 2.36                     | 0.55              |
| 36:2b:88:THR:O    | 36:2b:92:ARG:HG3   | 2.05                     | 0.55              |
| 47:2m:19:A:H2'    | 47:2m:20:G:O4'     | 2.06                     | 0.55              |
| 47:2m:96:C:H2'    | 47:2m:97:U:H6      | 1.68                     | 0.55              |
| 47:2m:453:C:O2'   | 70:3H:92:ARG:O     | 2.19                     | 0.55              |
| 47:2m:1409:A:H5'' | 58:2x:26:LYS:HD3   | 1.88                     | 0.55              |
| 50:2p:48:ILE:HB   | 50:2p:86:LEU:HD23  | 1.89                     | 0.55              |
| 50:2p:110:LEU:HG  | 50:2p:175:VAL:CG1  | 2.37                     | 0.55              |
| 50:2p:137:VAL:CG2 | 50:2p:185:LYS:HB2  | 2.36                     | 0.55              |
| 50:2p:163:PRO:O   | 50:2p:167:TYR:HB2  | 2.07                     | 0.55              |
| 54:2t:105:ASP:CG  | 54:2t:107:THR:HG23 | 2.32                     | 0.55              |
| 55:2u:95:ARG:HD3  | 55:2u:95:ARG:H     | 1.72                     | 0.55              |
| 57:2w:86:LEU:O    | 57:2w:90:VAL:HG23  | 2.06                     | 0.55              |
| 59:2y:78:ARG:HG2  | 59:2y:81:ARG:NH2   | 2.19                     | 0.55              |
| 59:2y:78:ARG:HA   | 59:2y:81:ARG:HE    | 1.71                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:3G:84:PHE:CZ    | 69:3G:264:SER:HA   | 2.40                     | 0.55              |
| 69:3G:109:ILE:HD13 | 69:3G:126:ALA:HA   | 1.88                     | 0.55              |
| 70:3H:58:LYS:NZ    | 70:3H:105:ASN:HA   | 2.22                     | 0.55              |
| 70:3H:154:ARG:O    | 70:3H:157:VAL:HG12 | 2.06                     | 0.55              |
| 77:3O:70:PRO:HA    | 77:3O:73:VAL:CG1   | 2.36                     | 0.55              |
| 1:1A:111:C:OP1     | 36:2b:110:LYS:HE2  | 2.07                     | 0.55              |
| 1:1A:139:G:H2'     | 1:1A:140:G:C8      | 2.41                     | 0.55              |
| 1:1A:277:G:O2'     | 37:2c:30:ARG:NH1   | 2.38                     | 0.55              |
| 1:1A:429:A:H2'     | 1:1A:430:G:H8      | 1.71                     | 0.55              |
| 1:1A:513:U:H1'     | 1:1A:516:C:H41     | 1.70                     | 0.55              |
| 1:1A:1273:G:C2'    | 1:1A:1274:A:H5'    | 2.35                     | 0.55              |
| 1:1A:2017:A:O2'    | 1:1A:2018:C:OP1    | 2.17                     | 0.55              |
| 1:1A:3633:C:H2'    | 1:1A:3634:G:C8     | 2.40                     | 0.55              |
| 1:1A:3920:U:H2'    | 1:1A:3921:U:H6     | 1.70                     | 0.55              |
| 3:1C:121:G:H2'     | 3:1C:122:G:C8      | 2.41                     | 0.55              |
| 7:1G:223:PHE:O     | 7:1G:227:ILE:HG12  | 2.07                     | 0.55              |
| 8:1H:67:ALA:HA     | 8:1H:69:TYR:CE2    | 2.41                     | 0.55              |
| 36:2b:37:THR:O     | 36:2b:37:THR:HG23  | 2.06                     | 0.55              |
| 39:2e:49:ASP:CB    | 39:2e:52:LYS:HG3   | 2.31                     | 0.55              |
| 47:2m:141:A:H4'    | 47:2m:142:C:C5'    | 2.33                     | 0.55              |
| 47:2m:398:A:H4'    | 47:2m:399:C:C5'    | 2.36                     | 0.55              |
| 47:2m:845:G:O2'    | 47:2m:846:G:H5'    | 2.06                     | 0.55              |
| 47:2m:1213:C:O2'   | 47:2m:1214:A:H5'   | 2.06                     | 0.55              |
| 47:2m:1533:A:H2    | 47:2m:1536:G:N3    | 2.04                     | 0.55              |
| 47:2m:1620:A:N3    | 47:2m:1620:A:H2'   | 2.20                     | 0.55              |
| 48:2n:34:MET:HE2   | 48:2n:149:ASN:O    | 2.07                     | 0.55              |
| 49:2o:100:PHE:HD2  | 49:2o:181:LEU:HD11 | 1.70                     | 0.55              |
| 50:2p:67:ARG:NH2   | 55:2u:95:ARG:HA    | 2.20                     | 0.55              |
| 57:2w:70:MET:HE3   | 57:2w:70:MET:N     | 2.21                     | 0.55              |
| 58:2x:107:GLU:O    | 58:2x:111:ILE:HG12 | 2.06                     | 0.55              |
| 61:20:133:ARG:HD3  | 61:20:134:ILE:CG2  | 2.37                     | 0.55              |
| 68:3F:299:PHE:CD1  | 68:3F:309:VAL:HG12 | 2.41                     | 0.55              |
| 70:3H:6:SER:OG     | 70:3H:13:GLN:HB3   | 2.06                     | 0.55              |
| 1:1A:910:G:O2'     | 1:1A:911:U:H5'     | 2.07                     | 0.55              |
| 1:1A:2000:G:H3'    | 1:1A:2000:G:N3     | 2.22                     | 0.55              |
| 1:1A:2465:C:H2'    | 1:1A:2466:G:O4'    | 2.06                     | 0.55              |
| 1:1A:2634:C:H2'    | 1:1A:2635:U:H6     | 1.71                     | 0.55              |
| 1:1A:2907:G:H4'    | 1:1A:3590:G:N1     | 2.20                     | 0.55              |
| 1:1A:3798:U:H2'    | 1:1A:3800:A:OP2    | 2.05                     | 0.55              |
| 1:1A:3856:A:H5''   | 18:2J:83:TRP:O     | 2.06                     | 0.55              |
| 1:1A:3911:C:H2'    | 1:1A:3912:U:C6     | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4371:G:O2'    | 1:1A:4372:U:OP2    | 2.23                     | 0.55              |
| 1:1A:4680:G:H2'    | 1:1A:4681:A:C8     | 2.40                     | 0.55              |
| 1:1A:4968:A:H2'    | 1:1A:4969:C:C6     | 2.41                     | 0.55              |
| 1:1A:5061:A:H4'    | 1:1A:5062:G:O5'    | 2.05                     | 0.55              |
| 2:1B:92:C:H2'      | 2:1B:93:G:H8       | 1.71                     | 0.55              |
| 8:1H:176:THR:HG23  | 8:1H:176:THR:O     | 2.06                     | 0.55              |
| 11:2C:7:ASN:HB3    | 11:2C:58:ASP:OD1   | 2.06                     | 0.55              |
| 12:2D:187:LYS:HG2  | 12:2D:187:LYS:O    | 2.05                     | 0.55              |
| 23:2O:65:ARG:HA    | 23:2O:69:LYS:O     | 2.07                     | 0.55              |
| 47:2m:156:G:H5''   | 70:3H:2:LYS:HE3    | 1.88                     | 0.55              |
| 47:2m:161:U:H3'    | 47:2m:162:C:C5'    | 2.35                     | 0.55              |
| 47:2m:733:C:H2'    | 47:2m:734:C:C1'    | 2.36                     | 0.55              |
| 47:2m:1053:C:O2'   | 47:2m:1054:G:H5'   | 2.06                     | 0.55              |
| 47:2m:1149:A:O2'   | 47:2m:1150:A:OP2   | 2.17                     | 0.55              |
| 47:2m:1421:A:N6    | 47:2m:1426:U:O4    | 2.39                     | 0.55              |
| 47:2m:1579:A:OP2   | 50:2p:7:LYS:HD2    | 2.06                     | 0.55              |
| 47:2m:1682:C:H4'   | 47:2m:1683:C:OP1   | 2.05                     | 0.55              |
| 48:2n:205:ARG:CB   | 48:2n:210:ILE:HD11 | 2.36                     | 0.55              |
| 50:2p:168:VAL:HG22 | 50:2p:189:MET:CB   | 2.36                     | 0.55              |
| 53:2s:10:LYS:HD2   | 53:2s:45:ILE:HD11  | 1.88                     | 0.55              |
| 57:2w:108:LYS:H    | 57:2w:111:MET:HE2  | 1.71                     | 0.55              |
| 58:2x:82:TYR:O     | 58:2x:86:GLN:HG2   | 2.06                     | 0.55              |
| 60:2z:23:ARG:HG2   | 77:3O:48:VAL:HG11  | 1.89                     | 0.55              |
| 60:2z:63:GLU:HA    | 60:2z:66:ARG:HG2   | 1.89                     | 0.55              |
| 63:3A:13:VAL:HG23  | 63:3A:13:VAL:O     | 2.07                     | 0.55              |
| 69:3G:110:MET:SD   | 69:3G:125:LYS:HE3  | 2.46                     | 0.55              |
| 69:3G:165:VAL:HG21 | 69:3G:217:ALA:CB   | 2.35                     | 0.55              |
| 69:3G:263:LYS:HG2  | 69:3G:267:GLN:OE1  | 2.06                     | 0.55              |
| 70:3H:121:ILE:H    | 70:3H:125:THR:CG2  | 2.20                     | 0.55              |
| 71:3I:28:GLU:CD    | 71:3I:40:LYS:HD3   | 2.31                     | 0.55              |
| 71:3I:87:LEU:HD12  | 71:3I:91:LYS:HE3   | 1.87                     | 0.55              |
| 74:3L:98:ARG:HB3   | 74:3L:132:VAL:HG23 | 1.88                     | 0.55              |
| 76:3N:6:THR:HG23   | 76:3N:28:LEU:HD13  | 1.87                     | 0.55              |
| 76:3N:117:VAL:O    | 76:3N:122:LYS:HE2  | 2.06                     | 0.55              |
| 77:3O:73:VAL:HG22  | 77:3O:79:ILE:HG13  | 1.88                     | 0.55              |
| 1:1A:513:U:H2'     | 1:1A:515:C:C5      | 2.41                     | 0.55              |
| 1:1A:518:G:N2      | 1:1A:643:C:H2'     | 2.22                     | 0.55              |
| 1:1A:1341:U:H2'    | 1:1A:1342:A:H8     | 1.70                     | 0.55              |
| 1:1A:1656:U:O2'    | 1:1A:3906:A:N1     | 2.31                     | 0.55              |
| 1:1A:1761:G:H3'    | 1:1A:1761:G:OP2    | 2.06                     | 0.55              |
| 1:1A:1772:C:H2'    | 1:1A:1773:U:H6     | 1.71                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2019:C:H4'    | 1:1A:2020:U:OP2    | 2.06                     | 0.55              |
| 1:1A:2718:U:H5''   | 1:1A:2719:C:H5'    | 1.88                     | 0.55              |
| 1:1A:4635:A:OP1    | 1:1A:4636:U:O2'    | 2.23                     | 0.55              |
| 1:1A:4896:G:O2'    | 1:1A:4897:G:P      | 2.63                     | 0.55              |
| 2:1B:12:U:OP2      | 2:1B:67:C:O2'      | 2.24                     | 0.55              |
| 2:1B:27:G:H2'      | 2:1B:28:C:C6       | 2.41                     | 0.55              |
| 11:2C:93:ARG:HD2   | 11:2C:143:GLU:HB3  | 1.89                     | 0.55              |
| 12:2D:63:GLU:H     | 12:2D:63:GLU:CD    | 2.13                     | 0.55              |
| 17:2I:65:ASN:OD1   | 17:2I:67:SER:OG    | 2.23                     | 0.55              |
| 17:2I:74:ARG:HD3   | 17:2I:146:GLY:HA3  | 1.88                     | 0.55              |
| 19:2K:23:ILE:HD12  | 45:2k:5:LEU:HD21   | 1.89                     | 0.55              |
| 21:2M:85:ASP:OD1   | 21:2M:90:THR:HB    | 2.07                     | 0.55              |
| 39:2e:23:VAL:HG23  | 39:2e:64:LEU:HD21  | 1.88                     | 0.55              |
| 47:2m:15:U:H2'     | 47:2m:16:G:O4'     | 2.06                     | 0.55              |
| 47:2m:93:U:H2'     | 47:2m:94:G:O4'     | 2.06                     | 0.55              |
| 47:2m:1278:A:H2'   | 47:2m:1279:C:H6    | 1.70                     | 0.55              |
| 47:2m:1406:G:H2'   | 47:2m:1407:U:O4'   | 2.07                     | 0.55              |
| 47:2m:1453:C:O2    | 47:2m:1453:C:H2'   | 2.06                     | 0.55              |
| 47:2m:1488:C:H3'   | 47:2m:1489:A:H5''  | 1.87                     | 0.55              |
| 47:2m:1630:A:O2'   | 47:2m:1631:U:H5'   | 2.07                     | 0.55              |
| 47:2m:1862:G:O6    | 65:3C:34:LYS:HE2   | 2.07                     | 0.55              |
| 48:2n:115:ALA:O    | 48:2n:117:ARG:NH2  | 2.40                     | 0.55              |
| 50:2p:69:LEU:HA    | 50:2p:72:VAL:HG22  | 1.88                     | 0.55              |
| 53:2s:91:HIS:ND1   | 53:2s:172:THR:HG21 | 2.21                     | 0.55              |
| 54:2t:161:LEU:HD12 | 54:2t:162:LEU:N    | 2.22                     | 0.55              |
| 57:2w:84:ILE:HD12  | 57:2w:85:ILE:N     | 2.21                     | 0.55              |
| 57:2w:107:ILE:HA   | 57:2w:111:MET:CE   | 2.37                     | 0.55              |
| 68:3F:279:SER:O    | 68:3F:279:SER:OG   | 2.20                     | 0.55              |
| 75:3M:114:GLU:OE1  | 75:3M:117:ARG:HD2  | 2.07                     | 0.55              |
| 78:3P:14:GLU:OE2   | 78:3P:18:LYS:HE3   | 2.07                     | 0.55              |
| 1:1A:481:G:O2'     | 1:1A:482:G:H5'     | 2.07                     | 0.55              |
| 1:1A:909:A:H2'     | 1:1A:910:G:H8      | 1.72                     | 0.55              |
| 1:1A:963:G:O2'     | 1:1A:964:A:O4'     | 2.18                     | 0.55              |
| 1:1A:1193:C:O2'    | 1:1A:1194:G:H5'    | 2.06                     | 0.55              |
| 1:1A:1906:U:H2'    | 1:1A:1907:A:H8     | 1.71                     | 0.55              |
| 1:1A:2385:U:H4'    | 20:2L:3:MET:HG2    | 1.88                     | 0.55              |
| 1:1A:2501:C:O2'    | 1:1A:2502:G:H5'    | 2.07                     | 0.55              |
| 1:1A:2882:A:H2'    | 1:1A:2883:G:H5'    | 1.89                     | 0.55              |
| 1:1A:3977:C:N4     | 1:1A:4035:G:OP1    | 2.39                     | 0.55              |
| 1:1A:4040:C:N4     | 1:1A:4042:G:N7     | 2.55                     | 0.55              |
| 1:1A:4054:C:N3     | 46:2l:207:LYS:HD3  | 2.22                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:2A:136:VAL:O    | 9:2A:136:VAL:HG23  | 2.06                     | 0.55              |
| 29:2U:79:TRP:CE3  | 29:2U:87:ARG:HG3   | 2.42                     | 0.55              |
| 46:2l:143:ASN:OD1 | 46:2l:148:VAL:HG13 | 2.07                     | 0.55              |
| 47:2m:218:U:O2    | 54:2t:184:ARG:NH2  | 2.39                     | 0.55              |
| 47:2m:311:C:H2'   | 47:2m:312:G:O4'    | 2.07                     | 0.55              |
| 47:2m:918:U:H2'   | 47:2m:919:A:O4'    | 2.06                     | 0.55              |
| 47:2m:1394:G:H5'  | 58:2x:126:ARG:HG3  | 1.87                     | 0.55              |
| 47:2m:1409:A:H5'  | 58:2x:24:HIS:ND1   | 2.20                     | 0.55              |
| 47:2m:1517:G:H2'  | 47:2m:1518:C:C2    | 2.42                     | 0.55              |
| 47:2m:1597:C:O2'  | 47:2m:1598:G:O4'   | 2.24                     | 0.55              |
| 47:2m:1797:U:H2'  | 47:2m:1798:C:C6    | 2.41                     | 0.55              |
| 47:2m:1816:G:O2'  | 47:2m:1817:G:H5'   | 2.06                     | 0.55              |
| 52:2r:35:LEU:HB3  | 52:2r:39:ILE:HD13  | 1.89                     | 0.55              |
| 54:2t:85:ALA:CB   | 56:2v:9:ALA:HB2    | 2.35                     | 0.55              |
| 54:2t:142:SER:O   | 54:2t:145:ILE:HG13 | 2.07                     | 0.55              |
| 64:3B:100:VAL:HB  | 64:3B:122:VAL:HG22 | 1.88                     | 0.55              |
| 77:3O:74:SER:HA   | 77:3O:79:ILE:CG2   | 2.37                     | 0.55              |
| 1:1A:190:G:H2'    | 1:1A:191:G:H8      | 1.71                     | 0.55              |
| 1:1A:982:U:H2'    | 1:1A:983:C:O4'     | 2.06                     | 0.55              |
| 1:1A:1247:U:H2'   | 1:1A:1248:C:C6     | 2.41                     | 0.55              |
| 1:1A:2386:U:H2'   | 1:1A:2387:G:H8     | 1.71                     | 0.55              |
| 1:1A:2411:C:H2'   | 1:1A:2412:A:H8     | 1.70                     | 0.55              |
| 1:1A:2446:C:H2'   | 1:1A:2447:U:C6     | 2.41                     | 0.55              |
| 1:1A:2494:U:H3'   | 1:1A:2495:U:C5     | 2.41                     | 0.55              |
| 1:1A:3610:A:H2'   | 1:1A:3611:A:H8     | 1.71                     | 0.55              |
| 1:1A:4453:C:H2'   | 1:1A:4454:G:O4'    | 2.06                     | 0.55              |
| 1:1A:5061:A:H4'   | 1:1A:5062:G:H5''   | 1.88                     | 0.55              |
| 4:1D:249:THR:HA   | 47:2m:1044:G:N7    | 2.21                     | 0.55              |
| 6:1F:134:PRO:HA   | 6:1F:150:LEU:HD22  | 1.89                     | 0.55              |
| 7:1G:111:ASN:N    | 7:1G:116:ASP:OD1   | 2.40                     | 0.55              |
| 7:1G:217:ASP:HA   | 7:1G:220:LYS:HD2   | 1.88                     | 0.55              |
| 8:1H:281:ILE:HD12 | 8:1H:281:ILE:O     | 2.07                     | 0.55              |
| 10:2B:162:ASP:HB3 | 10:2B:163:PRO:CD   | 2.28                     | 0.55              |
| 15:2G:12:VAL:O    | 15:2G:58:THR:OG1   | 2.19                     | 0.55              |
| 19:2K:147:GLU:OE1 | 19:2K:147:GLU:HA   | 2.06                     | 0.55              |
| 22:2N:82:GLY:HA3  | 30:2V:16:TRP:HB2   | 1.89                     | 0.55              |
| 23:2O:72:VAL:HG11 | 23:2O:83:LEU:HD11  | 1.87                     | 0.55              |
| 23:2O:107:LYS:C   | 23:2O:108:GLU:HG3  | 2.32                     | 0.55              |
| 43:2i:24:THR:HG22 | 43:2i:25:GLN:N     | 2.22                     | 0.55              |
| 46:2l:3:SER:HB2   | 46:2l:213:PRO:HD3  | 1.88                     | 0.55              |
| 46:2l:54:ARG:HG3  | 46:2l:154:THR:CB   | 2.34                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:318:A:OP2   | 70:3H:183:ARG:NH2  | 2.39                     | 0.55              |
| 47:2m:654:A:OP2   | 47:2m:655:A:O2'    | 2.11                     | 0.55              |
| 47:2m:672:A:N6    | 47:2m:1161:U:O2'   | 2.40                     | 0.55              |
| 47:2m:917:U:H2'   | 47:2m:918:U:C6     | 2.42                     | 0.55              |
| 47:2m:1289:U:C5   | 80:3R:97:LYS:HE2   | 2.42                     | 0.55              |
| 47:2m:1444:U:H2'  | 47:2m:1445:U:H6    | 1.72                     | 0.55              |
| 48:2n:68:ILE:HG23 | 48:2n:120:ARG:HH21 | 1.72                     | 0.55              |
| 48:2n:141:ASN:HB3 | 63:3A:29:HIS:O     | 2.07                     | 0.55              |
| 57:2w:127:LYS:HG3 | 57:2w:128:HIS:N    | 2.20                     | 0.55              |
| 68:3F:17:TRP:O    | 68:3F:36:ARG:N     | 2.40                     | 0.55              |
| 68:3F:59:LEU:HB3  | 68:3F:90:TRP:CE3   | 2.42                     | 0.55              |
| 69:3G:137:VAL:O   | 69:3G:162:ILE:HG13 | 2.07                     | 0.55              |
| 76:3N:82:ALA:O    | 76:3N:86:GLU:HB2   | 2.07                     | 0.55              |
| 77:3O:47:LEU:HB2  | 77:3O:78:LYS:O     | 2.06                     | 0.55              |
| 77:3O:96:LEU:O    | 77:3O:97:ILE:HD13  | 2.07                     | 0.55              |
| 1:1A:216:C:H5'    | 1:1A:219:G:N3      | 2.22                     | 0.55              |
| 1:1A:272:U:H2'    | 1:1A:273:U:H6      | 1.70                     | 0.55              |
| 1:1A:288:G:H2'    | 1:1A:289:C:H6      | 1.72                     | 0.55              |
| 1:1A:2332:A:H4'   | 1:1A:2333:G:OP1    | 2.05                     | 0.55              |
| 1:1A:3751:G:H21   | 1:1A:3775:A:H8     | 1.51                     | 0.55              |
| 1:1A:4093:G:H3'   | 1:1A:4093:G:N3     | 2.22                     | 0.55              |
| 1:1A:4967:A:H2'   | 1:1A:4968:A:H8     | 1.70                     | 0.55              |
| 6:1F:179:ASP:O    | 6:1F:183:VAL:HG23  | 2.07                     | 0.55              |
| 7:1G:79:TYR:O     | 7:1G:82:GLU:HG2    | 2.07                     | 0.55              |
| 8:1H:270:TYR:OH   | 15:2G:106:ASP:HB3  | 2.07                     | 0.55              |
| 47:2m:95:G:N2     | 47:2m:474:G:H5'    | 2.20                     | 0.55              |
| 47:2m:492:C:N4    | 47:2m:507:G:OP2    | 2.26                     | 0.55              |
| 47:2m:789:G:H2'   | 47:2m:790:C:O4'    | 2.07                     | 0.55              |
| 47:2m:976:G:H2'   | 47:2m:977:C:C6     | 2.42                     | 0.55              |
| 47:2m:1127:C:H5'' | 78:3P:17:ARG:NH2   | 2.22                     | 0.55              |
| 47:2m:1143:A:H2'  | 47:2m:1144:A:C8    | 2.41                     | 0.55              |
| 47:2m:1235:G:H21  | 57:2w:135:ALA:CB   | 2.19                     | 0.55              |
| 47:2m:1567:G:H5'  | 61:20:33:TRP:CZ3   | 2.41                     | 0.55              |
| 48:2n:39:TYR:HB2  | 48:2n:50:ASN:OD1   | 2.07                     | 0.55              |
| 52:2r:70:GLU:HA   | 52:2r:73:THR:HG22  | 1.89                     | 0.55              |
| 57:2w:37:TYR:HB3  | 57:2w:41:GLN:HB2   | 1.89                     | 0.55              |
| 59:2y:70:SER:OG   | 59:2y:73:LEU:HD23  | 2.06                     | 0.55              |
| 68:3F:231:ASP:OD1 | 68:3F:232:GLY:N    | 2.38                     | 0.55              |
| 69:3G:104:ASP:HB3 | 69:3G:130:ILE:CD1  | 2.35                     | 0.55              |
| 71:3I:151:LEU:O   | 71:3I:154:GLN:HB3  | 2.07                     | 0.55              |
| 76:3N:35:VAL:HG22 | 76:3N:40:ILE:HG12  | 1.89                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 80:3R:140:TYR:OH   | 80:3R:145:CYS:HA  | 2.06                     | 0.55              |
| 1:1A:121:A:H2      | 1:1A:152:U:H3     | 1.52                     | 0.55              |
| 1:1A:1703:C:H3'    | 1:1A:1704:C:C6    | 2.42                     | 0.55              |
| 1:1A:1953:U:H2'    | 1:1A:1954:U:C6    | 2.42                     | 0.55              |
| 1:1A:1968:G:H2'    | 1:1A:1969:G:O4'   | 2.07                     | 0.55              |
| 1:1A:2669:C:HO2'   | 1:1A:2670:C:H6    | 1.47                     | 0.55              |
| 1:1A:4084:G:O6     | 4:1D:68:ARG:HD2   | 2.06                     | 0.55              |
| 1:1A:4701:A:C2'    | 1:1A:4702:G:H5'   | 2.37                     | 0.55              |
| 1:1A:4871:C:H5'    | 15:2G:91:TRP:CE2  | 2.41                     | 0.55              |
| 12:2D:77:VAL:HG22  | 12:2D:82:ARG:HA   | 1.88                     | 0.55              |
| 13:2E:151:ILE:CD1  | 13:2E:156:ARG:HG2 | 2.26                     | 0.55              |
| 15:2G:132:LYS:HA   | 15:2G:135:LEU:CD2 | 2.36                     | 0.55              |
| 46:2L:28:PHE:CD1   | 46:2L:29:LEU:N    | 2.74                     | 0.55              |
| 46:2L:193:LEU:HG   | 46:2L:194:LEU:CD1 | 2.37                     | 0.55              |
| 47:2M:95:G:H21     | 47:2M:474:G:C5'   | 2.19                     | 0.55              |
| 47:2M:161:U:OP2    | 76:3N:116:LYS:HE3 | 2.07                     | 0.55              |
| 47:2M:1065:G:O2'   | 47:2M:1066:U:H5'  | 2.07                     | 0.55              |
| 47:2M:1103:C:H2'   | 47:2M:1104:G:C8   | 2.42                     | 0.55              |
| 47:2M:1422:G:H1'   | 47:2M:1424:G:C8   | 2.42                     | 0.55              |
| 59:2Y:58:MET:SD    | 59:2Y:61:ILE:HD11 | 2.47                     | 0.55              |
| 68:3F:154:VAL:HG22 | 68:3F:167:SER:CB  | 2.36                     | 0.55              |
| 69:3G:81:ILE:HG23  | 69:3G:86:LEU:HB2  | 1.89                     | 0.55              |
| 70:3H:63:MET:HE1   | 70:3H:98:ARG:C    | 2.31                     | 0.55              |
| 70:3H:140:ARG:HG2  | 70:3H:143:LYS:NZ  | 2.21                     | 0.55              |
| 71:3I:21:GLU:OE1   | 71:3I:21:GLU:HA   | 2.07                     | 0.55              |
| 1:1A:1084:C:H2'    | 1:1A:1085:C:C6    | 2.41                     | 0.55              |
| 1:1A:1699:A:N3     | 1:1A:1699:A:H2'   | 2.22                     | 0.55              |
| 1:1A:2375:A:O2'    | 1:1A:2376:A:H5'   | 2.06                     | 0.55              |
| 1:1A:2630:U:OP1    | 23:2O:48:LYS:NZ   | 2.40                     | 0.55              |
| 1:1A:3848:U:H2'    | 1:1A:3849:A:C8    | 2.42                     | 0.55              |
| 1:1A:4162:C:H5'    | 1:1A:4162:C:O2    | 2.07                     | 0.55              |
| 1:1A:4220:A:O2'    | 1:1A:4222:G:OP1   | 2.23                     | 0.55              |
| 1:1A:4379:A:H4'    | 43:2I:55:ILE:O    | 2.07                     | 0.55              |
| 1:1A:4758:U:O2'    | 1:1A:4759:C:H5'   | 2.07                     | 0.55              |
| 9:2A:93:ILE:HG21   | 9:2A:247:MET:HE2  | 1.89                     | 0.55              |
| 11:2C:137:SER:CB   | 11:2C:143:GLU:HG3 | 2.36                     | 0.55              |
| 14:2F:59:VAL:O     | 14:2F:70:VAL:HG22 | 2.07                     | 0.55              |
| 15:2G:33:GLN:HG2   | 15:2G:33:GLN:O    | 2.04                     | 0.55              |
| 16:2H:84:PRO:HA    | 16:2H:87:HIS:CD2  | 2.42                     | 0.55              |
| 17:2I:74:ARG:HH11  | 17:2I:74:ARG:HG3  | 1.71                     | 0.55              |
| 21:2M:84:TYR:CE1   | 21:2M:93:MET:HE3  | 2.42                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:2W:48:LEU:HD23  | 31:2W:93:THR:HB    | 1.87                     | 0.55              |
| 47:2m:302:A:H1'    | 54:2t:73:THR:HG21  | 1.87                     | 0.55              |
| 47:2m:317:C:H2'    | 47:2m:318:A:C8     | 2.41                     | 0.55              |
| 47:2m:795:A:H5'    | 47:2m:796:G:OP2    | 2.07                     | 0.55              |
| 47:2m:1680:G:O2'   | 47:2m:1681:U:H5'   | 2.07                     | 0.55              |
| 50:2p:25:LEU:HD13  | 50:2p:50:ILE:CD1   | 2.37                     | 0.55              |
| 54:2t:197:PHE:O    | 54:2t:201:LYS:HG2  | 2.06                     | 0.55              |
| 57:2w:43:ARG:O     | 57:2w:47:ARG:HG3   | 2.06                     | 0.55              |
| 57:2w:84:ILE:HD12  | 57:2w:85:ILE:H     | 1.72                     | 0.55              |
| 58:2x:66:VAL:HG13  | 58:2x:68:ILE:HD11  | 1.88                     | 0.55              |
| 62:21:40:ILE:HG22  | 62:21:44:LYS:NZ    | 2.22                     | 0.55              |
| 69:3G:204:ILE:HG23 | 69:3G:214:LEU:HD23 | 1.89                     | 0.55              |
| 73:3K:130:LYS:HE3  | 73:3K:137:PRO:O    | 2.08                     | 0.55              |
| 74:3L:21:VAL:HG12  | 74:3L:25:GLU:OE2   | 2.06                     | 0.55              |
| 78:3P:15:GLU:O     | 78:3P:23:ARG:NE    | 2.40                     | 0.55              |
| 1:1A:660:A:H2'     | 1:1A:661:C:O4'     | 2.06                     | 0.54              |
| 1:1A:1092:G:H2'    | 1:1A:1093:C:H6     | 1.72                     | 0.54              |
| 1:1A:1189:G:O2'    | 1:1A:1190:C:H5'    | 2.06                     | 0.54              |
| 1:1A:2413:U:H2'    | 1:1A:2414:G:H8     | 1.72                     | 0.54              |
| 1:1A:2753:G:O2'    | 1:1A:2754:G:H5'    | 2.07                     | 0.54              |
| 1:1A:4238:G:H2'    | 1:1A:4239:A:C8     | 2.43                     | 0.54              |
| 2:1B:73:U:OP2      | 2:1B:74:A:O2'      | 2.13                     | 0.54              |
| 14:2F:42:LYS:O     | 14:2F:46:ILE:HG12  | 2.07                     | 0.54              |
| 47:2m:360:A:C2     | 47:2m:362:C:H2'    | 2.42                     | 0.54              |
| 47:2m:1059:G:H2'   | 47:2m:1060:A:H5'   | 1.87                     | 0.54              |
| 47:2m:1287:A:H5''  | 47:2m:1288:U:C5    | 2.42                     | 0.54              |
| 47:2m:1318:G:H2'   | 47:2m:1319:U:O4'   | 2.07                     | 0.54              |
| 47:2m:1498:A:OP2   | 50:2p:27:ARG:NH1   | 2.40                     | 0.54              |
| 47:2m:1518:C:H5''  | 47:2m:1519:U:C5'   | 2.33                     | 0.54              |
| 47:2m:1770:G:OP1   | 47:2m:1771:G:H5'   | 2.07                     | 0.54              |
| 48:2n:42:LYS:HB2   | 48:2n:46:ILE:O     | 2.07                     | 0.54              |
| 55:2u:1:MET:HB3    | 55:2u:3:MET:CG     | 2.37                     | 0.54              |
| 55:2u:95:ARG:HD3   | 55:2u:95:ARG:N     | 2.20                     | 0.54              |
| 61:20:56:ARG:HG3   | 61:20:103:VAL:HG21 | 1.89                     | 0.54              |
| 64:3B:84:PHE:O     | 64:3B:86:PRO:HD3   | 2.07                     | 0.54              |
| 68:3F:121:VAL:HG23 | 68:3F:131:LEU:CD2  | 2.37                     | 0.54              |
| 68:3F:205:SER:C    | 68:3F:206:LEU:HD12 | 2.32                     | 0.54              |
| 68:3F:258:ILE:CG2  | 68:3F:267:VAL:HB   | 2.36                     | 0.54              |
| 69:3G:191:VAL:HG11 | 69:3G:236:PHE:HA   | 1.89                     | 0.54              |
| 77:3O:74:SER:OG    | 77:3O:79:ILE:HG22  | 2.06                     | 0.54              |
| 1:1A:295:A:OP2     | 43:2i:39:ARG:NH1   | 2.41                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:347:A:O2'    | 1:1A:348:G:H5'     | 2.07                     | 0.54              |
| 1:1A:448:G:H3'    | 1:1A:449:C:H5''    | 1.90                     | 0.54              |
| 1:1A:1970:A:H1'   | 1:1A:2018:C:H42    | 1.73                     | 0.54              |
| 1:1A:2255:C:O2    | 1:1A:2255:C:C2'    | 2.55                     | 0.54              |
| 1:1A:2730:U:H2'   | 1:1A:2731:C:C6     | 2.42                     | 0.54              |
| 1:1A:3807:A:O2'   | 1:1A:3808:C:H5'    | 2.06                     | 0.54              |
| 1:1A:3937:C:H1'   | 16:2H:125:SER:HB2  | 1.88                     | 0.54              |
| 1:1A:3944:G:N2    | 1:1A:4069:U:O2     | 2.25                     | 0.54              |
| 1:1A:4316:G:H2'   | 1:1A:4317:A:H5'    | 1.89                     | 0.54              |
| 1:1A:4344:U:H2'   | 1:1A:4345:C:C6     | 2.42                     | 0.54              |
| 1:1A:4442:U:O2'   | 1:1A:4443:C:H5'    | 2.07                     | 0.54              |
| 1:1A:4633:G:OP2   | 81:1A:5104:84D:N3  | 2.41                     | 0.54              |
| 1:1A:4745:G:N2    | 1:1A:4954:G:H22    | 2.05                     | 0.54              |
| 1:1A:4919:G:H2'   | 1:1A:4920:C:C6     | 2.41                     | 0.54              |
| 13:2E:136:ARG:HB2 | 13:2E:139:PHE:CE1  | 2.42                     | 0.54              |
| 14:2F:46:ILE:O    | 14:2F:46:ILE:HG13  | 2.06                     | 0.54              |
| 23:2O:65:ARG:O    | 23:2O:65:ARG:HG3   | 2.07                     | 0.54              |
| 36:2b:80:PRO:O    | 36:2b:84:ARG:HG3   | 2.07                     | 0.54              |
| 47:2m:418:A:HO2'  | 47:2m:419:G:P      | 2.29                     | 0.54              |
| 47:2m:696:G:C2'   | 47:2m:697:G:H5''   | 2.37                     | 0.54              |
| 47:2m:996:A:H5''  | 73:3K:7:PRO:CG     | 2.37                     | 0.54              |
| 47:2m:1224:G:O2'  | 47:2m:1225:U:H5'   | 2.08                     | 0.54              |
| 47:2m:1311:C:N4   | 47:2m:1312:G:O6    | 2.40                     | 0.54              |
| 47:2m:1743:G:H21  | 47:2m:1791:A:H62   | 1.54                     | 0.54              |
| 50:2p:39:VAL:HG12 | 50:2p:41:VAL:HG23  | 1.89                     | 0.54              |
| 51:2q:11:ARG:HD3  | 51:2q:21:ASP:O     | 2.07                     | 0.54              |
| 58:2x:16:LYS:C    | 58:2x:17:LYS:HG3   | 2.32                     | 0.54              |
| 59:2y:72:LYS:CG   | 59:2y:73:LEU:HD22  | 2.37                     | 0.54              |
| 60:2z:121:ARG:HD3 | 60:2z:131:VAL:HG21 | 1.87                     | 0.54              |
| 62:21:55:ARG:HG2  | 62:21:87:ARG:CZ    | 2.37                     | 0.54              |
| 68:3F:99:ARG:HG3  | 68:3F:100:ARG:N    | 2.21                     | 0.54              |
| 68:3F:212:LYS:HA  | 68:3F:235:ILE:HG23 | 1.89                     | 0.54              |
| 69:3G:199:PRO:O   | 69:3G:202:THR:OG1  | 2.18                     | 0.54              |
| 73:3K:46:THR:OG1  | 73:3K:49:GLN:HG3   | 2.07                     | 0.54              |
| 74:3L:82:ALA:O    | 74:3L:86:LYS:HG3   | 2.07                     | 0.54              |
| 80:3R:138:ARG:HB2 | 80:3R:148:TYR:O    | 2.07                     | 0.54              |
| 1:1A:82:U:O2'     | 1:1A:83:C:H5'      | 2.07                     | 0.54              |
| 1:1A:85:G:O2'     | 1:1A:97:G:O6       | 2.18                     | 0.54              |
| 1:1A:216:C:H4'    | 1:1A:219:G:H21     | 1.73                     | 0.54              |
| 1:1A:280:G:H5''   | 16:2H:14:LYS:CE    | 2.36                     | 0.54              |
| 1:1A:1247:U:H2'   | 1:1A:1248:C:H6     | 1.72                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2485:U:O3'   | 1:1A:2486:G:N2     | 2.41                     | 0.54              |
| 1:1A:2854:G:H4'   | 81:1A:5110:84D:O6  | 2.07                     | 0.54              |
| 1:1A:3648:A:H1'   | 1:1A:3785:A:N6     | 2.22                     | 0.54              |
| 1:1A:3916:G:H2'   | 1:1A:3917:A:C8     | 2.42                     | 0.54              |
| 1:1A:4454:G:HO2'  | 1:1A:4500:U:HO2'   | 1.55                     | 0.54              |
| 1:1A:4881:U:HO2'  | 1:1A:4882:U:H6     | 1.56                     | 0.54              |
| 1:1A:4888:U:H2'   | 1:1A:4889:G:C8     | 2.42                     | 0.54              |
| 1:1A:4961:G:O2'   | 1:1A:4962:C:H5'    | 2.06                     | 0.54              |
| 3:1C:111:U:OP2    | 40:2f:6:THR:HB     | 2.07                     | 0.54              |
| 7:1G:236:MET:HA   | 7:1G:239:MET:HE2   | 1.88                     | 0.54              |
| 11:2C:10:VAL:CG2  | 11:2C:78:GLN:HG3   | 2.37                     | 0.54              |
| 13:2E:82:ILE:HG22 | 13:2E:130:PHE:HE2  | 1.71                     | 0.54              |
| 13:2E:95:ARG:O    | 13:2E:98:ASN:HB2   | 2.07                     | 0.54              |
| 21:2M:29:ARG:HB3  | 22:2N:148:PRO:HB2  | 1.89                     | 0.54              |
| 23:2O:78:PHE:HE1  | 23:2O:83:LEU:HD13  | 1.71                     | 0.54              |
| 28:2T:11:VAL:HG12 | 28:2T:82:PRO:HA    | 1.89                     | 0.54              |
| 42:2h:7:LYS:HD3   | 42:2h:11:ARG:NH1   | 2.22                     | 0.54              |
| 42:2h:12:ARG:HG2  | 42:2h:15:ARG:NH2   | 2.23                     | 0.54              |
| 47:2m:1362:U:H5'' | 47:2m:1363:C:C5    | 2.42                     | 0.54              |
| 47:2m:1373:C:OP2  | 59:2y:7:LYS:HE3    | 2.07                     | 0.54              |
| 47:2m:1398:G:O3'  | 68:3F:88:ARG:NH2   | 2.41                     | 0.54              |
| 47:2m:1408:U:H5'' | 47:2m:1409:A:OP2   | 2.08                     | 0.54              |
| 47:2m:1576:G:O2'  | 47:2m:1577:G:H5'   | 2.07                     | 0.54              |
| 50:2p:140:GLY:HA3 | 50:2p:182:LEU:HD13 | 1.87                     | 0.54              |
| 52:2r:187:SER:O   | 52:2r:191:LYS:HG2  | 2.08                     | 0.54              |
| 53:2s:7:LYS:CE    | 53:2s:24:SER:HB3   | 2.23                     | 0.54              |
| 54:2t:118:ALA:O   | 54:2t:119:LEU:HD23 | 2.07                     | 0.54              |
| 56:2v:72:ILE:C    | 56:2v:73:LEU:HD23  | 2.33                     | 0.54              |
| 1:1A:113:A:H2'    | 1:1A:114:G:O4'     | 2.07                     | 0.54              |
| 1:1A:456:C:O2'    | 1:1A:457:G:OP2     | 2.23                     | 0.54              |
| 1:1A:496:G:C8     | 1:1A:498:C:H5''    | 2.42                     | 0.54              |
| 1:1A:2844:A:O2'   | 1:1A:4631:G:H4'    | 2.07                     | 0.54              |
| 4:1D:111:THR:O    | 4:1D:136:VAL:HG12  | 2.08                     | 0.54              |
| 11:2C:151:ILE:O   | 11:2C:155:SER:OG   | 2.24                     | 0.54              |
| 14:2F:47:ALA:CB   | 14:2F:48:PRO:HD3   | 2.30                     | 0.54              |
| 18:2J:23:ARG:O    | 18:2J:86:LYS:HE2   | 2.07                     | 0.54              |
| 23:2O:84:LYS:HB2  | 23:2O:110:TYR:CE2  | 2.42                     | 0.54              |
| 30:2V:25:ARG:NH1  | 30:2V:25:ARG:HA    | 2.22                     | 0.54              |
| 35:2a:46:CYS:O    | 35:2a:48:VAL:HG13  | 2.08                     | 0.54              |
| 45:2k:6:GLN:O     | 45:2k:10:VAL:HG22  | 2.06                     | 0.54              |
| 47:2m:65:C:C5     | 70:3H:174:PRO:HB3  | 2.42                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:750:C:N4     | 47:2m:794:A:H1'    | 2.17                     | 0.54              |
| 47:2m:1419:C:O5'   | 61:20:128:GLN:NE2  | 2.24                     | 0.54              |
| 47:2m:1458:G:OP1   | 68:3F:281:ALA:HB2  | 2.07                     | 0.54              |
| 47:2m:1493:C:H1'   | 47:2m:1498:A:N6    | 2.22                     | 0.54              |
| 47:2m:1641:A:H2'   | 47:2m:1642:U:O4'   | 2.07                     | 0.54              |
| 60:2z:121:ARG:HD3  | 60:2z:131:VAL:CG2  | 2.37                     | 0.54              |
| 65:3C:71:LEU:HD13  | 65:3C:73:TYR:OH    | 2.07                     | 0.54              |
| 66:3D:30:VAL:HB    | 66:3D:32:VAL:CG1   | 2.38                     | 0.54              |
| 68:3F:68:ASP:CG    | 68:3F:111:VAL:HG22 | 2.32                     | 0.54              |
| 68:3F:154:VAL:O    | 68:3F:155:ARG:HD3  | 2.07                     | 0.54              |
| 70:3H:216:ARG:C    | 70:3H:218:LYS:H    | 2.15                     | 0.54              |
| 71:3I:35:TYR:CD2   | 71:3I:106:LEU:HD13 | 2.42                     | 0.54              |
| 71:3I:59:GLU:OE1   | 71:3I:59:GLU:HA    | 2.08                     | 0.54              |
| 77:3O:100:VAL:CG2  | 77:3O:110:THR:HG22 | 2.37                     | 0.54              |
| 80:3R:102:VAL:HG21 | 80:3R:104:LYS:NZ   | 2.21                     | 0.54              |
| 1:1A:500:G:H4'     | 1:1A:504:G:OP2     | 2.08                     | 0.54              |
| 1:1A:679:C:H2'     | 1:1A:680:G:H8      | 1.72                     | 0.54              |
| 1:1A:1551:C:O2'    | 1:1A:1552:G:H5'    | 2.08                     | 0.54              |
| 1:1A:1596:U:O3'    | 18:2J:132:ALA:HB2  | 2.08                     | 0.54              |
| 1:1A:1775:A:H3'    | 1:1A:1776:A:H8     | 1.72                     | 0.54              |
| 1:1A:2631:U:H1'    | 23:2O:82:TYR:CD2   | 2.43                     | 0.54              |
| 1:1A:3605:C:OP2    | 20:2L:71:ARG:HG3   | 2.07                     | 0.54              |
| 1:1A:4301:U:OP1    | 22:2N:78:LYS:NZ    | 2.40                     | 0.54              |
| 1:1A:5005:G:N2     | 1:1A:5041:G:H1'    | 2.23                     | 0.54              |
| 2:1B:22:A:N3       | 2:1B:22:A:H2'      | 2.22                     | 0.54              |
| 3:1C:62:A:H4'      | 3:1C:63:U:O5'      | 2.06                     | 0.54              |
| 10:2B:102:TYR:OH   | 10:2B:208:ASN:HB2  | 2.08                     | 0.54              |
| 37:2c:45:ARG:HH11  | 37:2c:45:ARG:HG2   | 1.72                     | 0.54              |
| 47:2m:24:C:O2'     | 47:2m:25:A:O5'     | 2.25                     | 0.54              |
| 47:2m:39:A:H2'     | 47:2m:40:A:O4'     | 2.07                     | 0.54              |
| 47:2m:633:C:O2'    | 79:3Q:16:THR:HG21  | 2.08                     | 0.54              |
| 47:2m:881:G:H2'    | 47:2m:882:U:C5     | 2.42                     | 0.54              |
| 47:2m:1321:G:H2'   | 47:2m:1322:G:H5'   | 1.90                     | 0.54              |
| 47:2m:1418:C:H4'   | 47:2m:1419:C:C6    | 2.43                     | 0.54              |
| 47:2m:1589:A:O2'   | 47:2m:1590:C:H5'   | 2.06                     | 0.54              |
| 49:2o:137:LEU:HG   | 49:2o:215:VAL:HG22 | 1.88                     | 0.54              |
| 51:2q:42:LEU:HD13  | 51:2q:109:PHE:CD2  | 2.40                     | 0.54              |
| 52:2r:103:LEU:CD1  | 77:3O:67:LEU:HB2   | 2.37                     | 0.54              |
| 53:2s:64:VAL:CG1   | 53:2s:65:PRO:HD2   | 2.38                     | 0.54              |
| 53:2s:145:ARG:HB2  | 75:3M:51:GLU:OE1   | 2.06                     | 0.54              |
| 56:2v:73:LEU:HB3   | 56:2v:90:ARG:NH2   | 2.23                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:2w:21:ASP:OD1   | 57:2w:24:GLN:HB2   | 2.06                     | 0.54              |
| 58:2x:23:ALA:HB2   | 58:2x:70:VAL:HG22  | 1.88                     | 0.54              |
| 68:3F:47:ARG:HD3   | 68:3F:47:ARG:N     | 2.22                     | 0.54              |
| 68:3F:285:GLN:HB2  | 68:3F:303:THR:CG2  | 2.37                     | 0.54              |
| 70:3H:63:MET:HE1   | 70:3H:98:ARG:HB3   | 1.88                     | 0.54              |
| 70:3H:176:ILE:CG2  | 70:3H:179:LEU:HB2  | 2.37                     | 0.54              |
| 71:3I:80:ARG:O     | 71:3I:83:ARG:HG2   | 2.08                     | 0.54              |
| 74:3L:78:ALA:HB3   | 74:3L:118:ALA:HB3  | 1.88                     | 0.54              |
| 1:1A:384:A:N1      | 1:1A:405:U:H4'     | 2.22                     | 0.54              |
| 1:1A:483:G:C3'     | 1:1A:484:U:H5'     | 2.35                     | 0.54              |
| 1:1A:1762:C:HO2'   | 1:1A:1763:C:H6     | 1.53                     | 0.54              |
| 1:1A:2363:A:H2'    | 1:1A:2364:G:O4'    | 2.07                     | 0.54              |
| 1:1A:2411:C:H2'    | 1:1A:2412:A:C8     | 2.43                     | 0.54              |
| 1:1A:2520:C:O2     | 1:1A:2640:G:N2     | 2.40                     | 0.54              |
| 1:1A:4111:U:H2'    | 1:1A:4112:C:C1'    | 2.37                     | 0.54              |
| 1:1A:4370:G:H5''   | 43:2i:64:LYS:HG2   | 1.90                     | 0.54              |
| 3:1C:93:C:O2'      | 3:1C:94:G:H8       | 1.91                     | 0.54              |
| 12:2D:61:SER:HB2   | 12:2D:63:GLU:OE1   | 2.08                     | 0.54              |
| 19:2K:23:ILE:HD12  | 45:2k:5:LEU:CD2    | 2.37                     | 0.54              |
| 20:2L:172:ARG:CZ   | 47:2m:908:A:H5''   | 2.38                     | 0.54              |
| 25:2Q:101:ARG:HH12 | 70:3H:156:TYR:HE2  | 1.56                     | 0.54              |
| 26:2R:72:ASP:O     | 26:2R:76:ILE:HG13  | 2.06                     | 0.54              |
| 28:2T:99:ASP:O     | 28:2T:102:ARG:HG2  | 2.08                     | 0.54              |
| 32:2X:44:ARG:O     | 32:2X:48:GLU:HG2   | 2.07                     | 0.54              |
| 40:2f:27:ILE:HD13  | 40:2f:30:LYS:HD2   | 1.89                     | 0.54              |
| 47:2m:297:A:O2'    | 51:2q:135:GLY:HA2  | 2.07                     | 0.54              |
| 47:2m:338:G:H2'    | 47:2m:339:A:C8     | 2.42                     | 0.54              |
| 47:2m:460:A:H1'    | 47:2m:470:G:N2     | 2.22                     | 0.54              |
| 47:2m:925:G:O2'    | 47:2m:926:A:H5'    | 2.06                     | 0.54              |
| 47:2m:1657:G:O2'   | 67:3E:33:LYS:NZ    | 2.29                     | 0.54              |
| 47:2m:1839:U:H2'   | 47:2m:1840:U:H6    | 1.71                     | 0.54              |
| 48:2n:58:LEU:CD1   | 48:2n:161:ILE:HD13 | 2.33                     | 0.54              |
| 48:2n:137:ALA:HA   | 48:2n:142:LEU:CD2  | 2.37                     | 0.54              |
| 51:2q:48:LEU:CD1   | 51:2q:64:ILE:HD11  | 2.38                     | 0.54              |
| 51:2q:100:ARG:CB   | 51:2q:114:ILE:HD13 | 2.37                     | 0.54              |
| 55:2u:2:LEU:C      | 55:2u:3:MET:HG3    | 2.33                     | 0.54              |
| 58:2x:53:GLU:HB2   | 58:2x:54:PRO:HD3   | 1.88                     | 0.54              |
| 67:3E:2:GLY:CA     | 67:3E:6:LEU:HD11   | 2.30                     | 0.54              |
| 69:3G:125:LYS:CG   | 69:3G:143:CYS:HB2  | 2.33                     | 0.54              |
| 70:3H:140:ARG:CA   | 70:3H:143:LYS:HE2  | 2.38                     | 0.54              |
| 74:3L:12:GLU:HB3   | 74:3L:13:GLN:OE1   | 2.08                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 77:3O:107:VAL:O   | 77:3O:108:ILE:HD12 | 2.08                     | 0.54              |
| 1:1A:98:A:OP1     | 16:2H:195:ARG:HD3  | 2.08                     | 0.54              |
| 1:1A:197:A:O2'    | 1:1A:198:A:H5'     | 2.08                     | 0.54              |
| 1:1A:408:A:H5''   | 1:1A:409:G:OP1     | 2.08                     | 0.54              |
| 1:1A:1100:U:H1'   | 1:1A:1167:C:H42    | 1.73                     | 0.54              |
| 1:1A:1174:G:H21   | 7:1G:275:GLN:HE21  | 1.56                     | 0.54              |
| 1:1A:1378:C:H5    | 14:2F:159:ASN:H    | 1.56                     | 0.54              |
| 1:1A:1479:G:O2'   | 1:1A:1480:C:H5'    | 2.08                     | 0.54              |
| 1:1A:3684:G:H2'   | 1:1A:3685:C:C6     | 2.43                     | 0.54              |
| 1:1A:4137:C:H2'   | 1:1A:4138:C:H6     | 1.71                     | 0.54              |
| 1:1A:4869:U:H2'   | 1:1A:4870:G:C5'    | 2.37                     | 0.54              |
| 4:1D:130:SER:HB2  | 4:1D:171:GLY:HA3   | 1.88                     | 0.54              |
| 7:1G:108:ARG:NH2  | 7:1G:253:TYR:HB2   | 2.23                     | 0.54              |
| 11:2C:143:GLU:C   | 11:2C:144:LEU:HD23 | 2.33                     | 0.54              |
| 12:2D:107:GLY:HA2 | 12:2D:112:GLN:OE1  | 2.07                     | 0.54              |
| 15:2G:132:LYS:O   | 15:2G:135:LEU:HD23 | 2.07                     | 0.54              |
| 24:2P:40:ILE:HG12 | 24:2P:62:MET:O     | 2.08                     | 0.54              |
| 28:2T:10:VAL:CG2  | 28:2T:87:VAL:HG12  | 2.37                     | 0.54              |
| 32:2X:113:THR:OG1 | 32:2X:115:LYS:HG2  | 2.08                     | 0.54              |
| 35:2a:5:LEU:HD11  | 35:2a:22:LEU:HD22  | 1.90                     | 0.54              |
| 47:2m:85:A:H5''   | 76:3N:118:ARG:NE   | 2.22                     | 0.54              |
| 47:2m:857:U:H2'   | 47:2m:858:A:C8     | 2.42                     | 0.54              |
| 47:2m:872:A:O2'   | 47:2m:873:G:P      | 2.65                     | 0.54              |
| 47:2m:1262:C:N4   | 67:3E:15:GLY:HA3   | 2.22                     | 0.54              |
| 47:2m:1402:A:O5'  | 62:21:51:LYS:NZ    | 2.37                     | 0.54              |
| 47:2m:1528:G:H2'  | 47:2m:1529:C:C6    | 2.42                     | 0.54              |
| 47:2m:1606:G:H1'  | 47:2m:1633:A:N6    | 2.22                     | 0.54              |
| 47:2m:1745:A:H5'  | 47:2m:1746:U:OP2   | 2.07                     | 0.54              |
| 48:2n:111:GLN:HA  | 48:2n:116:PHE:CD2  | 2.43                     | 0.54              |
| 51:2q:97:GLU:HB3  | 51:2q:99:PHE:CE1   | 2.43                     | 0.54              |
| 52:2r:68:ILE:HD12 | 52:2r:69:VAL:N     | 2.22                     | 0.54              |
| 52:2r:193:LYS:HD2 | 52:2r:197:GLU:HG2  | 1.90                     | 0.54              |
| 60:2z:13:LEU:O    | 60:2z:20:ILE:N     | 2.41                     | 0.54              |
| 62:21:101:ILE:O   | 62:21:104:ILE:HG22 | 2.08                     | 0.54              |
| 70:3H:41:LEU:HD23 | 70:3H:41:LEU:H     | 1.72                     | 0.54              |
| 72:3J:50:CYS:HB3  | 72:3J:110:VAL:HG23 | 1.89                     | 0.54              |
| 76:3N:111:LYS:CG  | 76:3N:114:MET:HE3  | 2.38                     | 0.54              |
| 1:1A:429:A:H2'    | 1:1A:430:G:C8      | 2.43                     | 0.54              |
| 1:1A:476:G:O2'    | 1:1A:477:C:H5'     | 2.07                     | 0.54              |
| 1:1A:481:G:H2'    | 1:1A:482:G:C8      | 2.43                     | 0.54              |
| 1:1A:920:C:O2'    | 1:1A:921:C:H5'     | 2.08                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2494:U:H3'   | 1:1A:2495:U:C6     | 2.43                     | 0.54              |
| 1:1A:2738:C:O2'   | 1:1A:2740:U:O2     | 2.25                     | 0.54              |
| 1:1A:3635:A:C2    | 1:1A:3636:C:H1'    | 2.43                     | 0.54              |
| 1:1A:3939:G:O2'   | 1:1A:4076:G:N1     | 2.33                     | 0.54              |
| 1:1A:3967:G:H2'   | 1:1A:3968:U:C6     | 2.43                     | 0.54              |
| 1:1A:4238:G:O2'   | 1:1A:4239:A:H5'    | 2.08                     | 0.54              |
| 1:1A:4344:U:H2'   | 1:1A:4345:C:H6     | 1.72                     | 0.54              |
| 1:1A:4767:C:OP1   | 17:2I:168:TYR:OH   | 2.24                     | 0.54              |
| 3:1C:145:C:O2'    | 3:1C:146:U:H5'     | 2.08                     | 0.54              |
| 22:2N:144:ASN:HB2 | 22:2N:146:LYS:HE2  | 1.90                     | 0.54              |
| 25:2Q:76:VAL:HG12 | 25:2Q:77:LYS:N     | 2.23                     | 0.54              |
| 30:2V:51:LYS:HD3  | 30:2V:52:LYS:H     | 1.73                     | 0.54              |
| 35:2a:110:GLN:C   | 35:2a:110:GLN:OE1  | 2.50                     | 0.54              |
| 47:2m:65:C:C4     | 70:3H:174:PRO:HG3  | 2.42                     | 0.54              |
| 47:2m:107:A:H2'   | 47:2m:108:G:H8     | 1.70                     | 0.54              |
| 47:2m:213:G:HO2'  | 47:2m:214:U:P      | 2.29                     | 0.54              |
| 47:2m:411:G:O2'   | 47:2m:412:G:H5'    | 2.08                     | 0.54              |
| 47:2m:996:A:H2'   | 47:2m:997:A:H8     | 1.71                     | 0.54              |
| 47:2m:1398:G:H4'  | 68:3F:61:GLY:O     | 2.08                     | 0.54              |
| 50:2p:193:ASP:OD2 | 50:2p:198:ILE:HG22 | 2.08                     | 0.54              |
| 52:2r:193:LYS:NZ  | 52:2r:194:ASP:OD1  | 2.22                     | 0.54              |
| 54:2t:90:LEU:HA   | 54:2t:93:THR:OG1   | 2.07                     | 0.54              |
| 61:20:63:HIS:HE1  | 61:20:78:ILE:HD12  | 1.71                     | 0.54              |
| 65:3C:10:ARG:HB3  | 65:3C:34:LYS:HB2   | 1.89                     | 0.54              |
| 66:3D:30:VAL:HB   | 66:3D:32:VAL:HG13  | 1.90                     | 0.54              |
| 76:3N:38:THR:O    | 76:3N:41:ARG:HG2   | 2.08                     | 0.54              |
| 76:3N:102:THR:HB  | 76:3N:106:GLN:NE2  | 2.23                     | 0.54              |
| 1:1A:38:A:H5''    | 29:2U:35:ALA:CB    | 2.37                     | 0.54              |
| 1:1A:106:A:O2'    | 1:1A:107:G:H5'     | 2.08                     | 0.54              |
| 1:1A:217:C:H5     | 1:1A:219:G:H4'     | 1.73                     | 0.54              |
| 1:1A:451:C:H3'    | 1:1A:1294:A:H2     | 1.71                     | 0.54              |
| 1:1A:702:U:C2'    | 1:1A:703:G:H4'     | 2.33                     | 0.54              |
| 1:1A:1356:U:O2'   | 1:1A:1357:C:H5'    | 2.07                     | 0.54              |
| 1:1A:3619:G:H4'   | 20:2L:79:GLY:O     | 2.08                     | 0.54              |
| 1:1A:3765:G:C2'   | 1:1A:3766:A:H5'    | 2.35                     | 0.54              |
| 1:1A:3930:U:H2'   | 1:1A:3931:C:H6     | 1.73                     | 0.54              |
| 1:1A:4130:C:H2'   | 1:1A:4131:G:H8     | 1.71                     | 0.54              |
| 1:1A:4452:U:H4'   | 1:1A:4453:C:OP1    | 2.07                     | 0.54              |
| 1:1A:4637:G:H2'   | 1:1A:4638:U:H6     | 1.71                     | 0.54              |
| 2:1B:23:A:O2'     | 2:1B:24:C:H6       | 1.91                     | 0.54              |
| 4:1D:177:LYS:HD2  | 44:2j:29:ILE:HG21  | 1.88                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:1D:179:ILE:O    | 4:1D:180:LEU:HB2   | 2.08                     | 0.54              |
| 10:2B:81:ASN:O    | 10:2B:84:THR:OG1   | 2.25                     | 0.54              |
| 47:2m:312:G:H5'   | 47:2m:313:A:P      | 2.48                     | 0.54              |
| 47:2m:421:G:OP1   | 56:2v:98:LYS:HA    | 2.07                     | 0.54              |
| 47:2m:636:C:H2'   | 47:2m:637:U:O4'    | 2.08                     | 0.54              |
| 47:2m:1204:A:H2'  | 47:2m:1205:C:O4'   | 2.08                     | 0.54              |
| 47:2m:1326:U:O4   | 67:3E:28:HIS:ND1   | 2.38                     | 0.54              |
| 47:2m:1391:C:H4'  | 67:3E:55:LEU:CD2   | 2.34                     | 0.54              |
| 47:2m:1601:A:H1'  | 47:2m:1604:G:O6    | 2.08                     | 0.54              |
| 48:2n:158:ASP:O   | 63:3A:66:ASP:HA    | 2.08                     | 0.54              |
| 50:2p:193:ASP:HB3 | 50:2p:199:GLY:CA   | 2.37                     | 0.54              |
| 52:2r:73:THR:O    | 52:2r:89:THR:HG21  | 2.07                     | 0.54              |
| 55:2u:20:VAL:HG12 | 55:2u:70:TYR:HA    | 1.90                     | 0.54              |
| 58:2x:60:LYS:HD3  | 58:2x:64:ALA:HB2   | 1.90                     | 0.54              |
| 59:2y:23:ARG:O    | 59:2y:34:VAL:HG11  | 2.07                     | 0.54              |
| 59:2y:60:ARG:O    | 59:2y:63:ARG:HG2   | 2.07                     | 0.54              |
| 60:2z:54:LYS:HE3  | 60:2z:58:GLU:CB    | 2.38                     | 0.54              |
| 60:2z:142:ARG:HD2 | 60:2z:142:ARG:C    | 2.33                     | 0.54              |
| 71:3I:44:TRP:O    | 71:3I:47:LYS:HG2   | 2.08                     | 0.54              |
| 74:3L:130:GLU:HA  | 74:3L:130:GLU:OE1  | 2.08                     | 0.54              |
| 1:1A:158:A:N1     | 1:1A:276:C:O2'     | 2.39                     | 0.54              |
| 1:1A:255:C:N4     | 1:1A:256:G:N7      | 2.55                     | 0.54              |
| 1:1A:702:U:H3'    | 1:1A:703:G:C5'     | 2.38                     | 0.54              |
| 1:1A:1242:G:C2'   | 30:2V:120:ARG:HH21 | 2.21                     | 0.54              |
| 1:1A:1359:G:H4'   | 16:2H:203:TYR:HB2  | 1.89                     | 0.54              |
| 1:1A:1521:C:O2'   | 1:1A:1522:G:H5'    | 2.08                     | 0.54              |
| 1:1A:4460:U:H2'   | 1:1A:4461:C:H6     | 1.71                     | 0.54              |
| 6:1F:236:ASN:HB3  | 6:1F:239:LYS:HG3   | 1.90                     | 0.54              |
| 10:2B:164:ILE:O   | 10:2B:164:ILE:HG23 | 2.07                     | 0.54              |
| 19:2K:154:LYS:HB3 | 19:2K:161:SER:HB2  | 1.90                     | 0.54              |
| 23:2O:42:PHE:CD2  | 23:2O:90:TYR:HB2   | 2.43                     | 0.54              |
| 26:2R:52:LEU:HD12 | 26:2R:54:LEU:HD23  | 1.89                     | 0.54              |
| 35:2a:46:CYS:HB3  | 35:2a:86:CYS:SG    | 2.48                     | 0.54              |
| 47:2m:162:C:OP1   | 47:2m:162:C:H3'    | 2.08                     | 0.54              |
| 47:2m:490:C:O2'   | 47:2m:491:C:H5'    | 2.07                     | 0.54              |
| 47:2m:494:C:N4    | 47:2m:495:U:O4     | 2.41                     | 0.54              |
| 47:2m:799:U:O2'   | 47:2m:800:U:H5'    | 2.07                     | 0.54              |
| 47:2m:953:C:O2    | 74:3L:55:ARG:NH2   | 2.40                     | 0.54              |
| 47:2m:1425:G:HO2' | 47:2m:1426:U:P     | 2.30                     | 0.54              |
| 47:2m:1609:C:H3'  | 60:2z:132:ARG:HH21 | 1.72                     | 0.54              |
| 48:2n:79:SER:HA   | 48:2n:101:GLY:O    | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:2q:44:LEU:HD22  | 51:2q:72:ILE:HD11  | 1.90                     | 0.54              |
| 53:2s:126:HIS:CE1  | 53:2s:181:THR:HG23 | 2.43                     | 0.54              |
| 53:2s:130:LEU:HD13 | 53:2s:177:TYR:CD1  | 2.41                     | 0.54              |
| 59:2y:17:ILE:CD1   | 59:2y:54:VAL:HG13  | 2.38                     | 0.54              |
| 62:21:61:LEU:HD23  | 67:3E:34:TYR:CZ    | 2.42                     | 0.54              |
| 68:3F:201:SER:HA   | 68:3F:241:PHE:CD2  | 2.43                     | 0.54              |
| 69:3G:204:ILE:CG2  | 69:3G:214:LEU:HD23 | 2.38                     | 0.54              |
| 77:3O:47:LEU:HD22  | 77:3O:79:ILE:CD1   | 2.30                     | 0.54              |
| 79:3Q:24:LYS:HD2   | 79:3Q:25:LYS:O     | 2.08                     | 0.54              |
| 1:1A:444:G:H2'     | 1:1A:445:U:H6      | 1.72                     | 0.53              |
| 1:1A:758:G:H5'     | 11:2C:51:LYS:NZ    | 2.23                     | 0.53              |
| 1:1A:950:G:H2'     | 1:1A:951:G:H8      | 1.73                     | 0.53              |
| 1:1A:1208:G:O2'    | 1:1A:1209:U:H5'    | 2.08                     | 0.53              |
| 1:1A:1415:G:C2'    | 1:1A:1416:G:H5'    | 2.38                     | 0.53              |
| 1:1A:1695:U:H2'    | 1:1A:1696:C:C6     | 2.43                     | 0.53              |
| 1:1A:1698:C:O2'    | 1:1A:1699:A:O5'    | 2.19                     | 0.53              |
| 1:1A:1783:C:O2'    | 1:1A:1784:U:H5'    | 2.07                     | 0.53              |
| 1:1A:3849:A:O2'    | 1:1A:3850:C:H5'    | 2.08                     | 0.53              |
| 1:1A:3965:A:N7     | 1:1A:4049:U:O2'    | 2.37                     | 0.53              |
| 2:1B:115:A:O2'     | 2:1B:116:G:H5'     | 2.08                     | 0.53              |
| 3:1C:81:C:H5'      | 36:2b:3:LYS:HZ1    | 1.73                     | 0.53              |
| 6:1F:32:ILE:O      | 19:2K:23:ILE:HD11  | 2.08                     | 0.53              |
| 18:2J:32:THR:HG22  | 18:2J:91:LEU:HD12  | 1.90                     | 0.53              |
| 18:2J:95:LEU:HD23  | 18:2J:148:MET:SD   | 2.48                     | 0.53              |
| 21:2M:29:ARG:NH2   | 22:2N:150:LEU:HD12 | 2.24                     | 0.53              |
| 44:2j:28:LYS:HE2   | 44:2j:28:LYS:HA    | 1.90                     | 0.53              |
| 45:2k:54:ALA:HA    | 45:2k:61:VAL:HG23  | 1.90                     | 0.53              |
| 47:2m:539:C:H5'    | 47:2m:540:U:H4'    | 1.90                     | 0.53              |
| 47:2m:641:A:H2'    | 47:2m:642:U:O4'    | 2.08                     | 0.53              |
| 47:2m:689:U:H2'    | 47:2m:690:G:O4'    | 2.07                     | 0.53              |
| 47:2m:1533:A:N7    | 47:2m:1602:U:O4    | 2.41                     | 0.53              |
| 47:2m:1616:U:O2    | 47:2m:1661:A:H2    | 1.90                     | 0.53              |
| 47:2m:1650:A:H3'   | 47:2m:1651:A:H8    | 1.72                     | 0.53              |
| 47:2m:1661:A:C8    | 67:3E:14:PHE:HB2   | 2.43                     | 0.53              |
| 48:2n:111:GLN:HA   | 48:2n:116:PHE:HE2  | 1.73                     | 0.53              |
| 50:2p:70:THR:HG22  | 50:2p:86:LEU:HD12  | 1.90                     | 0.53              |
| 52:2r:18:LYS:HG3   | 52:2r:18:LYS:O     | 2.07                     | 0.53              |
| 57:2w:60:LEU:HG    | 57:2w:89:MET:SD    | 2.47                     | 0.53              |
| 57:2w:108:LYS:N    | 57:2w:111:MET:HE2  | 2.23                     | 0.53              |
| 67:3E:39:CYS:SG    | 67:3E:42:CYS:N     | 2.75                     | 0.53              |
| 76:3N:111:LYS:HA   | 76:3N:114:MET:HE3  | 1.89                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:19:G:O2'      | 1:1A:20:U:H5'      | 2.08                     | 0.53              |
| 1:1A:130:C:H2'     | 1:1A:131:C:H1'     | 1.88                     | 0.53              |
| 1:1A:174:C:O2'     | 1:1A:175:C:H5'     | 2.09                     | 0.53              |
| 1:1A:512:U:C2'     | 1:1A:513:U:H5'     | 2.38                     | 0.53              |
| 1:1A:963:G:H3'     | 1:1A:963:G:N3      | 2.23                     | 0.53              |
| 1:1A:1187:G:H21    | 1:1A:1187:G:P      | 2.26                     | 0.53              |
| 1:1A:1730:U:H2'    | 1:1A:1731:C:H6     | 1.72                     | 0.53              |
| 1:1A:2517:A:H5'    | 35:2a:62:LYS:HE3   | 1.90                     | 0.53              |
| 1:1A:2696:A:H5'    | 39:2e:26:LYS:HE2   | 1.91                     | 0.53              |
| 7:1G:217:ASP:HA    | 7:1G:220:LYS:CG    | 2.38                     | 0.53              |
| 8:1H:179:LEU:HD12  | 8:1H:183:ARG:HA    | 1.89                     | 0.53              |
| 11:2C:36:ARG:HG2   | 11:2C:38:PHE:CZ    | 2.43                     | 0.53              |
| 12:2D:76:MET:HE1   | 12:2D:148:VAL:CG1  | 2.32                     | 0.53              |
| 12:2D:182:GLU:OE1  | 12:2D:182:GLU:HA   | 2.08                     | 0.53              |
| 16:2H:16:SER:CB    | 37:2c:48:CYS:HB2   | 2.38                     | 0.53              |
| 27:2S:37:GLU:H     | 27:2S:37:GLU:CD    | 2.13                     | 0.53              |
| 46:2l:59:PRO:HB3   | 46:2l:170:GLY:CA   | 2.37                     | 0.53              |
| 46:2l:175:THR:OG1  | 46:2l:176:ASP:N    | 2.41                     | 0.53              |
| 46:2l:212:LYS:HE2  | 46:2l:214:GLN:OE1  | 2.08                     | 0.53              |
| 47:2m:77:A:O4'     | 70:3H:154:ARG:HB3  | 2.08                     | 0.53              |
| 47:2m:147:A:HO2'   | 47:2m:148:U:H6     | 1.56                     | 0.53              |
| 47:2m:337:C:C3'    | 47:2m:338:G:H4'    | 2.37                     | 0.53              |
| 47:2m:425:G:H4'    | 47:2m:427:U:O4     | 2.08                     | 0.53              |
| 47:2m:446:G:P      | 54:2t:47:ARG:HH12  | 2.31                     | 0.53              |
| 47:2m:797:C:O3'    | 47:2m:798:A:H4'    | 2.08                     | 0.53              |
| 47:2m:987:A:OP2    | 47:2m:988:C:N4     | 2.35                     | 0.53              |
| 48:2n:63:ARG:HG2   | 48:2n:185:MET:CE   | 2.37                     | 0.53              |
| 49:2o:49:VAL:CG1   | 49:2o:58:ALA:HB1   | 2.38                     | 0.53              |
| 50:2p:25:LEU:HD13  | 50:2p:37:VAL:HG11  | 1.89                     | 0.53              |
| 50:2p:63:GLY:O     | 50:2p:67:ARG:HD3   | 2.09                     | 0.53              |
| 52:2r:28:VAL:HG11  | 52:2r:109:LEU:HB2  | 1.90                     | 0.53              |
| 52:2r:112:LEU:HD13 | 52:2r:177:LEU:CD1  | 2.37                     | 0.53              |
| 53:2s:144:ILE:HG13 | 53:2s:154:ILE:CG1  | 2.23                     | 0.53              |
| 54:2t:161:LEU:HD13 | 54:2t:195:LEU:CD2  | 2.38                     | 0.53              |
| 57:2w:72:LYS:HZ2   | 57:2w:93:MET:HB2   | 1.73                     | 0.53              |
| 58:2x:93:VAL:HG22  | 58:2x:108:ILE:HD12 | 1.90                     | 0.53              |
| 70:3H:38:ALA:HB1   | 70:3H:41:LEU:HD21  | 1.90                     | 0.53              |
| 70:3H:181:THR:HG23 | 70:3H:183:ARG:N    | 2.23                     | 0.53              |
| 71:3I:61:LEU:CD2   | 71:3I:94:LEU:HG    | 2.37                     | 0.53              |
| 80:3R:120:GLU:O    | 80:3R:132:MET:HE3  | 2.08                     | 0.53              |
| 1:1A:438:G:C2'     | 1:1A:439:G:H5'     | 2.38                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1298:C:H2'    | 1:1A:1299:G:C8     | 2.43                     | 0.53              |
| 1:1A:1708:G:O2'    | 1:1A:1709:C:H5'    | 2.08                     | 0.53              |
| 1:1A:2056:G:H5''   | 17:2I:128:ARG:NH2  | 2.23                     | 0.53              |
| 1:1A:2292:C:H2'    | 1:1A:2293:U:C6     | 2.44                     | 0.53              |
| 1:1A:2526:C:OP2    | 20:2L:38:ARG:HG3   | 2.08                     | 0.53              |
| 1:1A:4093:G:O2'    | 1:1A:4094:G:O4'    | 2.23                     | 0.53              |
| 1:1A:4099:G:O2'    | 1:1A:4111:U:N3     | 2.24                     | 0.53              |
| 3:1C:122:G:O6      | 3:1C:128:C:N4      | 2.41                     | 0.53              |
| 5:1E:57:VAL:HG22   | 5:1E:73:VAL:HG22   | 1.89                     | 0.53              |
| 7:1G:219:TYR:CE2   | 7:1G:227:ILE:HD11  | 2.44                     | 0.53              |
| 15:2G:118:MET:HG3  | 17:2I:192:TYR:CE2  | 2.44                     | 0.53              |
| 19:2K:50:ARG:CA    | 19:2K:53:MET:HG3   | 2.31                     | 0.53              |
| 23:2O:69:LYS:NZ    | 23:2O:69:LYS:HB3   | 2.22                     | 0.53              |
| 23:2O:91:LEU:HD13  | 23:2O:96:LEU:CB    | 2.39                     | 0.53              |
| 28:2T:123:LYS:O    | 28:2T:124:THR:HG23 | 2.08                     | 0.53              |
| 47:2m:389:A:O2'    | 47:2m:390:C:H5'    | 2.07                     | 0.53              |
| 47:2m:481:C:H2'    | 47:2m:482:G:C1'    | 2.38                     | 0.53              |
| 47:2m:628:A:H61    | 50:2p:141:LYS:HZ1  | 1.55                     | 0.53              |
| 47:2m:835:C:N4     | 76:3N:9:THR:HG22   | 2.23                     | 0.53              |
| 47:2m:948:C:O2'    | 47:2m:949:G:H5'    | 2.09                     | 0.53              |
| 47:2m:1102:G:H22   | 47:2m:1130:G:N2    | 2.06                     | 0.53              |
| 47:2m:1414:A:H3'   | 47:2m:1414:A:OP1   | 2.08                     | 0.53              |
| 47:2m:1670:C:H2'   | 47:2m:1671:G:C8    | 2.43                     | 0.53              |
| 49:2o:174:ARG:O    | 49:2o:174:ARG:HD3  | 2.07                     | 0.53              |
| 51:2q:66:MET:O     | 51:2q:68:ARG:HG3   | 2.08                     | 0.53              |
| 52:2r:18:LYS:HE2   | 52:2r:18:LYS:HA    | 1.88                     | 0.53              |
| 57:2w:98:ASN:O     | 57:2w:122:THR:HG22 | 2.07                     | 0.53              |
| 58:2x:66:VAL:CG1   | 58:2x:68:ILE:HD11  | 2.39                     | 0.53              |
| 67:3E:53:ILE:O     | 67:3E:55:LEU:HD12  | 2.09                     | 0.53              |
| 68:3F:18:VAL:HG21  | 68:3F:307:VAL:HG23 | 1.91                     | 0.53              |
| 68:3F:79:LEU:CD2   | 68:3F:87:LEU:HD22  | 2.38                     | 0.53              |
| 69:3G:78:LEU:HD12  | 69:3G:81:ILE:HD12  | 1.91                     | 0.53              |
| 69:3G:205:VAL:HG21 | 69:3G:223:TYR:CE1  | 2.43                     | 0.53              |
| 70:3H:2:LYS:HB3    | 70:3H:15:LEU:HD21  | 1.91                     | 0.53              |
| 70:3H:35:GLU:HG3   | 70:3H:51:ARG:HB2   | 1.89                     | 0.53              |
| 71:3I:39:ASN:HA    | 79:3Q:34:ARG:NH1   | 2.22                     | 0.53              |
| 72:3J:114:TYR:CE2  | 72:3J:120:ALA:HB1  | 2.43                     | 0.53              |
| 73:3K:86:GLU:HG3   | 73:3K:87:ASP:N     | 2.23                     | 0.53              |
| 80:3R:140:TYR:CD1  | 80:3R:147:THR:HB   | 2.43                     | 0.53              |
| 1:1A:127:G:C2'     | 1:1A:128:C:H5'     | 2.36                     | 0.53              |
| 1:1A:418:A:H62     | 3:1C:16:G:H1'      | 1.73                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:468:U:N3      | 1:1A:686:A:N1      | 2.57                     | 0.53              |
| 1:1A:1089:G:O2'    | 1:1A:1090:G:H5'    | 2.08                     | 0.53              |
| 1:1A:1278:C:H2'    | 1:1A:1279:A:O4'    | 2.08                     | 0.53              |
| 1:1A:1440:U:H5''   | 1:1A:1441:C:OP1    | 2.09                     | 0.53              |
| 1:1A:1552:G:O2'    | 1:1A:1574:G:N2     | 2.33                     | 0.53              |
| 1:1A:2528:G:H3'    | 1:1A:2528:G:N3     | 2.23                     | 0.53              |
| 1:1A:3720:G:H22    | 1:1A:3733:A:H2     | 1.57                     | 0.53              |
| 1:1A:3760:A:H2'    | 1:1A:3760:A:N3     | 2.22                     | 0.53              |
| 1:1A:3975:C:OP2    | 46:2l:27:LYS:HB2   | 2.08                     | 0.53              |
| 1:1A:4185:G:O2'    | 1:1A:4186:A:H5'    | 2.08                     | 0.53              |
| 1:1A:4369:A:H4'    | 43:2i:67:VAL:CG2   | 2.39                     | 0.53              |
| 1:1A:4430:G:H1'    | 12:2D:158:LYS:HD2  | 1.89                     | 0.53              |
| 1:1A:4909:A:H2'    | 5:1E:156:TYR:CE1   | 2.44                     | 0.53              |
| 3:1C:154:G:H2'     | 3:1C:155:C:C6      | 2.42                     | 0.53              |
| 5:1E:96:PRO:HD3    | 17:2I:156:LEU:CD1  | 2.38                     | 0.53              |
| 5:1E:121:ASN:CG    | 5:1E:124:LYS:HG3   | 2.34                     | 0.53              |
| 5:1E:285:TYR:CD1   | 5:1E:363:ILE:HD13  | 2.43                     | 0.53              |
| 20:2L:183:GLU:O    | 20:2L:184:ILE:HD13 | 2.08                     | 0.53              |
| 24:2P:87:SER:HA    | 24:2P:97:TYR:HB3   | 1.90                     | 0.53              |
| 31:2W:23:LYS:HD2   | 31:2W:23:LYS:C     | 2.33                     | 0.53              |
| 47:2m:153:G:H21    | 70:3H:13:GLN:NE2   | 2.07                     | 0.53              |
| 47:2m:335:G:H2'    | 47:2m:336:A:O4'    | 2.09                     | 0.53              |
| 47:2m:816:A:C2'    | 47:2m:817:G:H5'    | 2.38                     | 0.53              |
| 47:2m:1144:A:H2'   | 47:2m:1145:A:C8    | 2.43                     | 0.53              |
| 47:2m:1476:A:C2    | 52:2r:59:LYS:HE2   | 2.44                     | 0.53              |
| 49:2o:150:ILE:HD13 | 59:2y:132:ARG:HH12 | 1.73                     | 0.53              |
| 50:2p:54:ARG:CG    | 50:2p:57:ASN:HB2   | 2.38                     | 0.53              |
| 50:2p:217:ILE:HG13 | 50:2p:218:LEU:H    | 1.73                     | 0.53              |
| 51:2q:100:ARG:NH2  | 51:2q:121:TYR:O    | 2.41                     | 0.53              |
| 52:2r:32:ASP:OD2   | 52:2r:35:LEU:HB2   | 2.09                     | 0.53              |
| 52:2r:73:THR:HG23  | 52:2r:86:LYS:HE3   | 1.90                     | 0.53              |
| 54:2t:36:THR:HG23  | 54:2t:57:ALA:O     | 2.09                     | 0.53              |
| 62:21:21:ARG:O     | 62:21:115:THR:HG22 | 2.08                     | 0.53              |
| 64:3B:24:ASP:OD1   | 64:3B:24:ASP:N     | 2.36                     | 0.53              |
| 68:3F:38:LYS:HB3   | 68:3F:62:HIS:O     | 2.09                     | 0.53              |
| 69:3G:62:PRO:HD3   | 69:3G:71:LYS:HD3   | 1.90                     | 0.53              |
| 70:3H:55:GLY:N     | 70:3H:63:MET:HG2   | 2.24                     | 0.53              |
| 71:3I:94:LEU:HD12  | 71:3I:97:ILE:CD1   | 2.35                     | 0.53              |
| 77:3O:57:LYS:HA    | 77:3O:60:LYS:CD    | 2.38                     | 0.53              |
| 1:1A:2:G:H2'       | 1:1A:3:C:C6        | 2.44                     | 0.53              |
| 1:1A:742:G:O2'     | 1:1A:743:G:H5'     | 2.08                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1070:G:O2'   | 1:1A:1071:C:O5'    | 2.26                     | 0.53              |
| 1:1A:1904:G:C2'   | 1:1A:1905:U:H5'    | 2.39                     | 0.53              |
| 1:1A:1920:C:O2'   | 1:1A:1922:G:H5''   | 2.09                     | 0.53              |
| 5:1E:45:ALA:HB1   | 5:1E:181:MET:HE1   | 1.90                     | 0.53              |
| 10:2B:129:PRO:O   | 10:2B:130:THR:OG1  | 2.15                     | 0.53              |
| 12:2D:146:GLU:H   | 12:2D:146:GLU:CD   | 2.11                     | 0.53              |
| 16:2H:115:VAL:HA  | 16:2H:134:LEU:HD13 | 1.90                     | 0.53              |
| 18:2J:29:THR:HG21 | 18:2J:146:ILE:HD11 | 1.89                     | 0.53              |
| 46:2I:54:ARG:HG2  | 46:2I:152:LYS:CD   | 2.31                     | 0.53              |
| 47:2m:339:A:H5''  | 47:2m:340:C:C5     | 2.43                     | 0.53              |
| 47:2m:825:A:O2'   | 47:2m:826:A:H5'    | 2.07                     | 0.53              |
| 47:2m:852:G:N3    | 47:2m:852:G:H2'    | 2.24                     | 0.53              |
| 47:2m:1387:G:C2   | 47:2m:1388:A:H1'   | 2.43                     | 0.53              |
| 47:2m:1566:G:N2   | 47:2m:1568:C:H2'   | 2.24                     | 0.53              |
| 47:2m:1587:G:C6   | 61:20:67:ARG:HD2   | 2.43                     | 0.53              |
| 47:2m:1606:G:H22  | 47:2m:1632:G:H2'   | 1.74                     | 0.53              |
| 52:2r:162:ALA:CB  | 52:2r:169:ILE:HA   | 2.39                     | 0.53              |
| 58:2x:28:GLY:HA3  | 58:2x:67:ASP:CG    | 2.34                     | 0.53              |
| 58:2x:102:GLU:OE1 | 58:2x:106:LYS:HD3  | 2.09                     | 0.53              |
| 58:2x:104:SER:O   | 58:2x:108:ILE:HG23 | 2.09                     | 0.53              |
| 60:2z:67:VAL:HA   | 60:2z:70:ILE:CG1   | 2.39                     | 0.53              |
| 67:3E:53:ILE:CD1  | 67:3E:55:LEU:HD11  | 2.38                     | 0.53              |
| 68:3F:116:ASP:HB3 | 68:3F:118:ARG:CZ   | 2.39                     | 0.53              |
| 69:3G:268:GLU:HG2 | 69:3G:269:PHE:CE1  | 2.44                     | 0.53              |
| 70:3H:109:LEU:CD2 | 70:3H:111:LEU:HG   | 2.38                     | 0.53              |
| 1:1A:911:U:O2'    | 1:1A:912:G:H5'     | 2.08                     | 0.53              |
| 1:1A:1700:G:H5'   | 1:1A:1702:C:OP2    | 2.09                     | 0.53              |
| 1:1A:2702:C:O2'   | 1:1A:2703:G:H5'    | 2.09                     | 0.53              |
| 1:1A:2756:G:H2'   | 1:1A:2757:A:C8     | 2.43                     | 0.53              |
| 1:1A:2840:A:C2'   | 1:1A:2841:G:H5'    | 2.39                     | 0.53              |
| 1:1A:3593:C:H3'   | 1:1A:3595:U:O4     | 2.08                     | 0.53              |
| 1:1A:4194:U:H5'   | 30:2V:3:LYS:HD3    | 1.91                     | 0.53              |
| 1:1A:4263:C:H2'   | 1:1A:4264:G:O4'    | 2.08                     | 0.53              |
| 1:1A:4464:A:H2'   | 1:1A:4464:A:N3     | 2.22                     | 0.53              |
| 1:1A:4504:C:H2'   | 1:1A:4505:C:H6     | 1.71                     | 0.53              |
| 1:1A:4638:U:H2'   | 1:1A:4639:G:N3     | 2.24                     | 0.53              |
| 5:1E:94:GLU:HG2   | 5:1E:99:LEU:CD1    | 2.39                     | 0.53              |
| 32:2X:57:MET:HE2  | 32:2X:88:LEU:HB2   | 1.90                     | 0.53              |
| 39:2e:59:SER:O    | 39:2e:59:SER:OG    | 2.26                     | 0.53              |
| 43:2i:23:VAL:HG22 | 43:2i:70:LEU:CD2   | 2.38                     | 0.53              |
| 47:2m:67:C:H5     | 70:3H:162:LEU:HD13 | 1.73                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:71:G:O2'    | 47:2m:72:C:OP1     | 2.20                     | 0.53              |
| 47:2m:589:G:H21   | 47:2m:591:U:H3     | 1.55                     | 0.53              |
| 47:2m:838:G:H1'   | 47:2m:840:C:OP2    | 2.08                     | 0.53              |
| 47:2m:860:G:H2'   | 75:3M:107:SER:OG   | 2.08                     | 0.53              |
| 47:2m:1007:C:H2'  | 47:2m:1008:A:H8    | 1.73                     | 0.53              |
| 47:2m:1143:A:H2'  | 47:2m:1144:A:N9    | 2.24                     | 0.53              |
| 47:2m:1545:A:O2'  | 47:2m:1546:G:H5''  | 2.08                     | 0.53              |
| 47:2m:1620:A:H4'  | 47:2m:1621:U:H5    | 1.73                     | 0.53              |
| 50:2p:9:ARG:HA    | 50:2p:12:VAL:HG22  | 1.89                     | 0.53              |
| 50:2p:76:ARG:HG3  | 55:2u:22:VAL:CG1   | 2.35                     | 0.53              |
| 60:2z:92:ASP:OD2  | 60:2z:94:LYS:HB2   | 2.08                     | 0.53              |
| 68:3F:68:ASP:OD1  | 68:3F:111:VAL:HG22 | 2.08                     | 0.53              |
| 68:3F:116:ASP:HB3 | 68:3F:118:ARG:CD   | 2.37                     | 0.53              |
| 69:3G:114:LYS:HD2 | 69:3G:121:ARG:NH2  | 2.23                     | 0.53              |
| 69:3G:172:ASN:O   | 69:3G:174:ILE:HG13 | 2.08                     | 0.53              |
| 75:3M:36:ARG:O    | 75:3M:40:VAL:HG23  | 2.09                     | 0.53              |
| 76:3N:111:LYS:C   | 76:3N:114:MET:HE3  | 2.34                     | 0.53              |
| 78:3P:35:VAL:CG1  | 78:3P:44:THR:HB    | 2.39                     | 0.53              |
| 80:3R:120:GLU:HG2 | 80:3R:131:PHE:CD1  | 2.43                     | 0.53              |
| 1:1A:716:C:OP1    | 6:1F:317:ASN:HB2   | 2.09                     | 0.53              |
| 1:1A:1836:G:OP1   | 22:2N:129:LYS:NZ   | 2.41                     | 0.53              |
| 1:1A:4141:G:O2'   | 1:1A:4143:G:N7     | 2.42                     | 0.53              |
| 1:1A:4375:C:H5''  | 1:1A:4376:A:OP1    | 2.08                     | 0.53              |
| 1:1A:4617:G:OP2   | 5:1E:358:ARG:NH2   | 2.25                     | 0.53              |
| 3:1C:12:G:H5''    | 18:2J:3:ARG:HG3    | 1.90                     | 0.53              |
| 6:1F:158:VAL:HG22 | 6:1F:170:LEU:HD22  | 1.91                     | 0.53              |
| 8:1H:117:PRO:O    | 45:2k:112:ARG:HD2  | 2.08                     | 0.53              |
| 13:2E:100:SER:OG  | 13:2E:131:TYR:OH   | 2.25                     | 0.53              |
| 14:2F:143:GLU:O   | 14:2F:147:ALA:HB2  | 2.09                     | 0.53              |
| 47:2m:79:A:H2'    | 47:2m:80:G:H5'     | 1.89                     | 0.53              |
| 47:2m:551:U:H3'   | 47:2m:552:G:C8     | 2.43                     | 0.53              |
| 47:2m:1144:A:O2'  | 47:2m:1145:A:H5'   | 2.09                     | 0.53              |
| 47:2m:1309:C:N4   | 80:3R:100:LEU:HD11 | 2.24                     | 0.53              |
| 47:2m:1397:U:N3   | 47:2m:1442:U:O4'   | 2.42                     | 0.53              |
| 47:2m:1616:U:H2'  | 47:2m:1617:G:O4'   | 2.08                     | 0.53              |
| 48:2n:155:ARG:HG2 | 48:2n:156:TYR:CE2  | 2.44                     | 0.53              |
| 51:2q:72:ILE:HD12 | 51:2q:77:ARG:CB    | 2.39                     | 0.53              |
| 56:2v:37:TYR:CE2  | 56:2v:51:ILE:HG12  | 2.44                     | 0.53              |
| 57:2w:67:ALA:HB2  | 57:2w:73:PRO:CB    | 2.39                     | 0.53              |
| 62:21:23:THR:HG22 | 62:21:88:LEU:HG    | 1.90                     | 0.53              |
| 69:3G:113:GLN:HG2 | 69:3G:122:THR:HG22 | 1.89                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:3G:135:GLY:O    | 69:3G:165:VAL:N    | 2.36                     | 0.53              |
| 69:3G:156:ILE:HG13 | 69:3G:157:LEU:N    | 2.22                     | 0.53              |
| 76:3N:7:ILE:CD1    | 76:3N:27:VAL:HG22  | 2.30                     | 0.53              |
| 76:3N:11:LYS:HB2   | 76:3N:24:VAL:CG2   | 2.39                     | 0.53              |
| 1:1A:343:C:O2'     | 1:1A:344:A:H5'     | 2.09                     | 0.53              |
| 1:1A:1182:C:H3'    | 1:1A:1182:C:OP2    | 2.08                     | 0.53              |
| 1:1A:1296:G:H2'    | 1:1A:1297:U:H6     | 1.74                     | 0.53              |
| 1:1A:1349:G:OP2    | 19:2K:54:SER:HB2   | 2.08                     | 0.53              |
| 1:1A:1707:C:O2     | 30:2V:102:PRO:HB2  | 2.09                     | 0.53              |
| 1:1A:2721:G:C2'    | 1:1A:2722:G:H5'    | 2.39                     | 0.53              |
| 1:1A:3656:A:H2'    | 1:1A:3657:U:C6     | 2.43                     | 0.53              |
| 1:1A:3845:A:H2'    | 1:1A:3846:C:C6     | 2.44                     | 0.53              |
| 1:1A:4048:A:H4'    | 1:1A:4048:A:OP1    | 2.09                     | 0.53              |
| 1:1A:4093:G:H2'    | 1:1A:4094:G:C8     | 2.44                     | 0.53              |
| 2:1B:4:U:H2'       | 2:1B:5:A:C8        | 2.44                     | 0.53              |
| 3:1C:144:U:H2'     | 3:1C:145:C:H6      | 1.73                     | 0.53              |
| 14:2F:57:PRO:HG3   | 14:2F:75:GLY:C     | 2.33                     | 0.53              |
| 14:2F:61:CYS:HB2   | 14:2F:66:TYR:O     | 2.09                     | 0.53              |
| 25:2Q:45:ASN:HB3   | 25:2Q:48:GLN:OE1   | 2.09                     | 0.53              |
| 26:2R:89:LYS:HG2   | 26:2R:95:THR:HG23  | 1.90                     | 0.53              |
| 26:2R:89:LYS:HG2   | 26:2R:95:THR:CG2   | 2.38                     | 0.53              |
| 27:2S:30:MET:HB3   | 27:2S:101:PRO:HG3  | 1.89                     | 0.53              |
| 47:2m:67:C:C6      | 70:3H:162:LEU:HD22 | 2.43                     | 0.53              |
| 47:2m:125:C:H2'    | 70:3H:198:ARG:CZ   | 2.39                     | 0.53              |
| 47:2m:433:A:H2'    | 47:2m:434:G:C8     | 2.43                     | 0.53              |
| 47:2m:510:G:O2'    | 47:2m:511:U:H5'    | 2.08                     | 0.53              |
| 47:2m:604:A:H1'    | 47:2m:639:C:O2'    | 2.09                     | 0.53              |
| 47:2m:636:C:O2'    | 47:2m:637:U:H5'    | 2.09                     | 0.53              |
| 47:2m:1404:U:C2    | 62:21:56:MET:HE3   | 2.44                     | 0.53              |
| 47:2m:1407:U:H3    | 47:2m:1440:C:H42   | 1.55                     | 0.53              |
| 47:2m:1648:G:N7    | 58:2x:17:LYS:HE3   | 2.23                     | 0.53              |
| 48:2n:30:LEU:HD12  | 48:2n:31:ASP:N     | 2.23                     | 0.53              |
| 48:2n:90:PHE:CD2   | 48:2n:179:ALA:HB2  | 2.43                     | 0.53              |
| 49:2o:36:PRO:HD3   | 49:2o:98:THR:HG23  | 1.89                     | 0.53              |
| 49:2o:110:MET:CA   | 49:2o:110:MET:HE3  | 2.39                     | 0.53              |
| 49:2o:198:GLU:OE2  | 49:2o:202:GLN:HG2  | 2.09                     | 0.53              |
| 53:2s:144:ILE:CG1  | 53:2s:154:ILE:HG13 | 2.24                     | 0.53              |
| 56:2v:72:ILE:O     | 56:2v:73:LEU:HD23  | 2.09                     | 0.53              |
| 57:2w:57:LEU:HG    | 57:2w:89:MET:HE1   | 1.90                     | 0.53              |
| 58:2x:32:ILE:CD1   | 58:2x:68:ILE:HG13  | 2.37                     | 0.53              |
| 60:2z:13:LEU:HD23  | 60:2z:20:ILE:CD1   | 2.30                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:2z:17:ASN:ND2   | 60:2z:101:ASN:HD21 | 2.07                     | 0.53              |
| 69:3G:213:LEU:HD21 | 69:3G:240:THR:HG21 | 1.90                     | 0.53              |
| 70:3H:12:CYS:O     | 70:3H:124:LEU:HA   | 2.08                     | 0.53              |
| 70:3H:181:THR:CG2  | 70:3H:184:VAL:H    | 2.21                     | 0.53              |
| 71:3I:143:ASN:C    | 71:3I:144:ILE:HG12 | 2.34                     | 0.53              |
| 76:3N:10:ARG:HG3   | 76:3N:24:VAL:HB    | 1.89                     | 0.53              |
| 76:3N:40:ILE:HD12  | 76:3N:60:PHE:CE2   | 2.43                     | 0.53              |
| 1:1A:382:G:H4'     | 1:1A:407:A:N1      | 2.24                     | 0.53              |
| 1:1A:479:G:H2'     | 1:1A:480:C:C6      | 2.44                     | 0.53              |
| 1:1A:1672:U:H2'    | 1:1A:1673:U:C6     | 2.44                     | 0.53              |
| 1:1A:1802:A:H4'    | 22:2N:105:PHE:CE1  | 2.44                     | 0.53              |
| 1:1A:1879:C:O2'    | 1:1A:1880:G:H5'    | 2.09                     | 0.53              |
| 1:1A:2258:C:O2     | 8:1H:91:THR:HG23   | 2.09                     | 0.53              |
| 1:1A:2439:G:H5'    | 1:1A:2778:G:OP2    | 2.09                     | 0.53              |
| 1:1A:2639:U:HO2'   | 1:1A:2640:G:P      | 2.32                     | 0.53              |
| 1:1A:3600:G:H2'    | 1:1A:3601:C:H6     | 1.74                     | 0.53              |
| 1:1A:4886:C:H2'    | 1:1A:4887:C:H5'    | 1.91                     | 0.53              |
| 4:1D:229:ALA:HB3   | 4:1D:234:LYS:HB3   | 1.91                     | 0.53              |
| 14:2F:7:GLY:O      | 29:2U:49:HIS:NE2   | 2.38                     | 0.53              |
| 46:2l:172:VAL:O    | 46:2l:174:MET:HG3  | 2.09                     | 0.53              |
| 47:2m:14:C:H5'     | 69:3G:190:SER:CB   | 2.39                     | 0.53              |
| 47:2m:1762:C:OP1   | 47:2m:1772:C:N4    | 2.36                     | 0.53              |
| 48:2n:103:PHE:CZ   | 48:2n:107:THR:HB   | 2.44                     | 0.53              |
| 50:2p:192:TRP:CZ2  | 50:2p:203:PRO:HG3  | 2.44                     | 0.53              |
| 51:2q:71:LYS:HA    | 51:2q:75:LYS:O     | 2.09                     | 0.53              |
| 51:2q:151:ASP:HB3  | 51:2q:154:ILE:HG13 | 1.91                     | 0.53              |
| 51:2q:175:PHE:HE1  | 51:2q:198:ARG:HG3  | 1.74                     | 0.53              |
| 54:2t:53:LYS:HE3   | 54:2t:55:TYR:CZ    | 2.44                     | 0.53              |
| 57:2w:116:LEU:HD12 | 57:2w:116:LEU:C    | 2.34                     | 0.53              |
| 58:2x:93:VAL:HG22  | 58:2x:108:ILE:CD1  | 2.39                     | 0.53              |
| 62:21:81:GLN:HG2   | 62:21:81:GLN:O     | 2.06                     | 0.53              |
| 68:3F:248:LEU:O    | 68:3F:248:LEU:HD12 | 2.08                     | 0.53              |
| 69:3G:125:LYS:HG3  | 69:3G:143:CYS:CB   | 2.33                     | 0.53              |
| 70:3H:231:ARG:HG2  | 70:3H:232:ARG:HD2  | 1.90                     | 0.53              |
| 71:3I:42:GLU:HG3   | 71:3I:45:ARG:NH2   | 2.24                     | 0.53              |
| 74:3L:71:PRO:O     | 74:3L:114:SER:OG   | 2.26                     | 0.53              |
| 75:3M:11:LEU:HD12  | 75:3M:74:VAL:HB    | 1.91                     | 0.53              |
| 76:3N:110:ARG:HG3  | 76:3N:130:LYS:HE3  | 1.91                     | 0.53              |
| 77:3O:49:LEU:H     | 77:3O:83:LEU:CD1   | 2.22                     | 0.53              |
| 80:3R:135:HIS:HB3  | 80:3R:138:ARG:NH1  | 2.23                     | 0.53              |
| 1:1A:934:C:H4'     | 1:1A:935:A:H5''    | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1175:A:H2     | 1:1A:1185:G:H1     | 1.57                     | 0.53              |
| 1:1A:1181:C:H3'    | 1:1A:1182:C:H5'    | 1.91                     | 0.53              |
| 1:1A:1759:G:C2'    | 1:1A:1760:G:H5'    | 2.39                     | 0.53              |
| 1:1A:1760:G:O3'    | 1:1A:1761:G:H2'    | 2.08                     | 0.53              |
| 1:1A:1929:A:H5'    | 1:1A:1930:U:OP1    | 2.08                     | 0.53              |
| 1:1A:4924:C:H2'    | 1:1A:4925:U:C6     | 2.44                     | 0.53              |
| 3:1C:103:A:OP2     | 3:1C:104:A:H2'     | 2.09                     | 0.53              |
| 7:1G:164:LYS:HA    | 7:1G:167:VAL:CG2   | 2.39                     | 0.53              |
| 19:2K:63:LEU:HD12  | 19:2K:66:MET:CE    | 2.39                     | 0.53              |
| 22:2N:27:LEU:HB3   | 22:2N:31:MET:HE3   | 1.91                     | 0.53              |
| 28:2T:29:ILE:HG22  | 28:2T:32:GLY:H     | 1.74                     | 0.53              |
| 41:2g:126:LYS:HB3  | 41:2g:128:LYS:HG3  | 1.90                     | 0.53              |
| 47:2m:385:G:H3'    | 56:2v:136:LYS:HB2  | 1.91                     | 0.53              |
| 47:2m:574:A:O2'    | 47:2m:575:A:O4'    | 2.27                     | 0.53              |
| 47:2m:692:G:N1     | 47:2m:739:C:N3     | 2.56                     | 0.53              |
| 47:2m:875:A:H5'    | 53:2s:111:LYS:NZ   | 2.24                     | 0.53              |
| 47:2m:901:G:O2'    | 47:2m:902:G:H5'    | 2.09                     | 0.53              |
| 47:2m:1543:U:H4'   | 58:2x:43:GLU:HG3   | 1.89                     | 0.53              |
| 48:2n:124:VAL:HG13 | 48:2n:130:ASP:HB2  | 1.90                     | 0.53              |
| 50:2p:141:LYS:CE   | 50:2p:179:GLN:HG2  | 2.39                     | 0.53              |
| 53:2s:130:LEU:HD22 | 53:2s:177:TYR:CZ   | 2.44                     | 0.53              |
| 54:2t:38:ILE:HA    | 54:2t:60:LEU:O     | 2.09                     | 0.53              |
| 57:2w:21:ASP:OD1   | 57:2w:21:ASP:N     | 2.41                     | 0.53              |
| 59:2y:46:LEU:O     | 59:2y:50:ILE:HG13  | 2.09                     | 0.53              |
| 60:2z:84:LEU:H     | 60:2z:84:LEU:HD12  | 1.73                     | 0.53              |
| 62:21:61:LEU:HD13  | 62:21:82:MET:HE2   | 1.91                     | 0.53              |
| 75:3M:5:ASN:HB3    | 75:3M:8:ALA:HB3    | 1.90                     | 0.53              |
| 77:3O:101:SER:OG   | 77:3O:108:ILE:HB   | 2.09                     | 0.53              |
| 1:1A:1196:G:O2'    | 1:1A:1197:C:H5'    | 2.09                     | 0.52              |
| 1:1A:1412:G:H2'    | 1:1A:1413:C:H6     | 1.74                     | 0.52              |
| 1:1A:1703:C:H5''   | 1:1A:1704:C:H5     | 1.74                     | 0.52              |
| 1:1A:2763:U:O2'    | 1:1A:2764:A:H5'    | 2.09                     | 0.52              |
| 1:1A:4092:G:C5     | 1:1A:4093:G:H8     | 2.27                     | 0.52              |
| 1:1A:4258:C:OP1    | 13:2E:53:ALA:HA    | 2.09                     | 0.52              |
| 81:1A:5103:84D:N2  | 81:1A:5103:84D:O7  | 2.42                     | 0.52              |
| 5:1E:109:HIS:HB2   | 5:1E:202:GLU:OE2   | 2.09                     | 0.52              |
| 11:2C:128:MET:HE1  | 11:2C:161:ILE:HG22 | 1.90                     | 0.52              |
| 19:2K:22:ASP:O     | 19:2K:26:ARG:HG2   | 2.09                     | 0.52              |
| 22:2N:74:ILE:HG22  | 22:2N:76:VAL:HG22  | 1.91                     | 0.52              |
| 28:2T:64:LYS:O     | 28:2T:67:LYS:HG3   | 2.09                     | 0.52              |
| 34:2Z:78:HIS:HB3   | 34:2Z:83:MET:O     | 2.09                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:525:A:OP2   | 79:3Q:26:LYS:NZ    | 2.31                     | 0.52              |
| 47:2m:696:G:H1'   | 47:2m:735:C:OP2    | 2.09                     | 0.52              |
| 47:2m:1166:G:O2'  | 47:2m:1167:G:H5'   | 2.09                     | 0.52              |
| 47:2m:1212:G:O2'  | 47:2m:1213:C:H5'   | 2.10                     | 0.52              |
| 47:2m:1288:U:H2'  | 47:2m:1289:U:C6    | 2.44                     | 0.52              |
| 47:2m:1323:U:O2'  | 47:2m:1324:G:H5'   | 2.09                     | 0.52              |
| 47:2m:1613:G:OP2  | 57:2w:39:ALA:N     | 2.42                     | 0.52              |
| 47:2m:1622:U:H3   | 57:2w:122:THR:HG1  | 1.57                     | 0.52              |
| 48:2n:157:VAL:CG1 | 48:2n:160:ALA:HB2  | 2.40                     | 0.52              |
| 49:2o:174:ARG:NH1 | 49:2o:178:THR:HG21 | 2.24                     | 0.52              |
| 50:2p:139:SER:HB2 | 50:2p:149:SER:HB2  | 1.89                     | 0.52              |
| 51:2q:178:GLY:O   | 51:2q:231:GLY:HA2  | 2.10                     | 0.52              |
| 52:2r:182:LYS:HE3 | 52:2r:184:SER:HB3  | 1.90                     | 0.52              |
| 53:2s:60:ILE:CD1  | 53:2s:90:LYS:HG2   | 2.39                     | 0.52              |
| 55:2u:91:PRO:HD2  | 55:2u:94:LEU:CD2   | 2.38                     | 0.52              |
| 57:2w:64:LYS:NZ   | 57:2w:90:VAL:O     | 2.31                     | 0.52              |
| 59:2y:77:GLU:O    | 59:2y:81:ARG:HG3   | 2.09                     | 0.52              |
| 61:20:71:GLY:O    | 61:20:75:MET:HG2   | 2.09                     | 0.52              |
| 68:3F:124:SER:O   | 68:3F:151:VAL:HB   | 2.09                     | 0.52              |
| 68:3F:292:SER:HB3 | 68:3F:297:THR:OG1  | 2.08                     | 0.52              |
| 70:3H:55:GLY:C    | 70:3H:63:MET:HG2   | 2.34                     | 0.52              |
| 71:3I:91:LYS:HG2  | 71:3I:96:TYR:CD2   | 2.44                     | 0.52              |
| 73:3K:33:VAL:HG21 | 73:3K:66:VAL:HG21  | 1.91                     | 0.52              |
| 1:1A:2:G:H2'      | 1:1A:3:C:H6        | 1.73                     | 0.52              |
| 1:1A:247:G:H2'    | 1:1A:248:C:C6      | 2.42                     | 0.52              |
| 1:1A:650:C:O2'    | 1:1A:651:C:H5'     | 2.10                     | 0.52              |
| 1:1A:661:C:H2'    | 1:1A:662:C:C5      | 2.43                     | 0.52              |
| 1:1A:978:G:OP1    | 8:1H:62:MET:HG3    | 2.09                     | 0.52              |
| 1:1A:987:C:H2'    | 1:1A:988:C:C6      | 2.45                     | 0.52              |
| 1:1A:1241:C:C5    | 30:2V:118:LEU:HD23 | 2.43                     | 0.52              |
| 1:1A:2056:G:H5''  | 17:2I:128:ARG:HH21 | 1.74                     | 0.52              |
| 1:1A:2505:C:H1'   | 1:1A:2506:G:N2     | 2.24                     | 0.52              |
| 1:1A:2727:C:H2'   | 1:1A:2728:U:C6     | 2.45                     | 0.52              |
| 1:1A:3652:A:H2'   | 1:1A:3653:A:C8     | 2.44                     | 0.52              |
| 1:1A:3786:U:O2    | 1:1A:3814:U:H4'    | 2.09                     | 0.52              |
| 1:1A:3953:G:H22   | 1:1A:4060:U:C1'    | 2.21                     | 0.52              |
| 1:1A:4413:C:H5    | 1:1A:4429:C:N4     | 2.07                     | 0.52              |
| 1:1A:4966:A:H2'   | 1:1A:4967:A:O4'    | 2.09                     | 0.52              |
| 3:1C:8:U:H2'      | 3:1C:9:A:C8        | 2.45                     | 0.52              |
| 3:1C:87:G:H2'     | 3:1C:87:G:OP2      | 2.10                     | 0.52              |
| 6:1F:76:ILE:HG13  | 6:1F:77:PRO:CD     | 2.40                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:2A:142:TRP:CZ2   | 9:2A:235:ASN:HB2   | 2.44                     | 0.52              |
| 10:2B:119:GLU:OE2  | 10:2B:120:LYS:HG2  | 2.08                     | 0.52              |
| 17:2I:85:ARG:HG3   | 17:2I:99:LEU:HD22  | 1.92                     | 0.52              |
| 24:2P:92:ASP:HB2   | 24:2P:94:VAL:HG12  | 1.92                     | 0.52              |
| 35:2a:41:ALA:O     | 35:2a:52:ARG:HD2   | 2.07                     | 0.52              |
| 36:2b:99:GLU:HA    | 36:2b:102:LEU:HD12 | 1.92                     | 0.52              |
| 46:2l:45:LYS:HG2   | 46:2l:46:ASP:N     | 2.21                     | 0.52              |
| 46:2l:65:VAL:HG12  | 46:2l:111:LEU:HD12 | 1.92                     | 0.52              |
| 47:2m:163:U:O3'    | 70:3H:83:CYS:HA    | 2.08                     | 0.52              |
| 47:2m:849:A:H2'    | 47:2m:850:C:O4'    | 2.10                     | 0.52              |
| 47:2m:1198:G:H2'   | 47:2m:1199:A:C8    | 2.44                     | 0.52              |
| 47:2m:1284:A:HO2'  | 72:3J:106:CYS:HA   | 1.72                     | 0.52              |
| 47:2m:1545:A:O2'   | 47:2m:1546:G:H8    | 1.92                     | 0.52              |
| 47:2m:1613:G:OP2   | 57:2w:38:SER:HA    | 2.08                     | 0.52              |
| 50:2p:26:THR:O     | 50:2p:30:ALA:HB2   | 2.08                     | 0.52              |
| 51:2q:36:HIS:CE1   | 51:2q:85:GLY:HA3   | 2.44                     | 0.52              |
| 51:2q:54:TYR:HD1   | 76:3N:13:MET:HE1   | 1.72                     | 0.52              |
| 52:2r:50:PRO:HB3   | 52:2r:69:VAL:HG12  | 1.90                     | 0.52              |
| 52:2r:100:ILE:HD11 | 52:2r:174:ALA:CA   | 2.38                     | 0.52              |
| 54:2t:26:LYS:O     | 54:2t:29:LEU:HG    | 2.08                     | 0.52              |
| 57:2w:33:LEU:CD1   | 57:2w:36:LEU:HD12  | 2.39                     | 0.52              |
| 57:2w:90:VAL:HA    | 57:2w:107:ILE:HG22 | 1.91                     | 0.52              |
| 58:2x:32:ILE:O     | 58:2x:33:LYS:HG3   | 2.09                     | 0.52              |
| 59:2y:66:VAL:O     | 59:2y:66:VAL:CG1   | 2.58                     | 0.52              |
| 60:2z:23:ARG:CZ    | 77:3O:48:VAL:HG21  | 2.39                     | 0.52              |
| 60:2z:28:PHE:O     | 60:2z:31:THR:OG1   | 2.15                     | 0.52              |
| 62:21:65:THR:HG23  | 62:21:67:LYS:H     | 1.74                     | 0.52              |
| 66:3D:34:PHE:O     | 66:3D:35:MET:HB3   | 2.08                     | 0.52              |
| 68:3F:62:HIS:CG    | 68:3F:82:SER:HB2   | 2.44                     | 0.52              |
| 68:3F:87:LEU:CD2   | 68:3F:111:VAL:HG11 | 2.30                     | 0.52              |
| 68:3F:194:TYR:O    | 68:3F:211:GLY:HA3  | 2.09                     | 0.52              |
| 69:3G:227:ARG:HG3  | 69:3G:228:GLY:N    | 2.24                     | 0.52              |
| 70:3H:140:ARG:HA   | 70:3H:143:LYS:CE   | 2.39                     | 0.52              |
| 70:3H:224:ARG:HG3  | 70:3H:224:ARG:HH11 | 1.74                     | 0.52              |
| 1:1A:425:U:H2'     | 1:1A:426:A:H8      | 1.75                     | 0.52              |
| 1:1A:967:C:H2'     | 1:1A:968:C:H5''    | 1.91                     | 0.52              |
| 1:1A:1077:C:C2'    | 1:1A:1078:A:H5'    | 2.39                     | 0.52              |
| 1:1A:2755:A:H2'    | 1:1A:2756:G:H5'    | 1.92                     | 0.52              |
| 1:1A:3960:A:H3'    | 1:1A:3961:G:C4'    | 2.40                     | 0.52              |
| 1:1A:4149:C:O2'    | 1:1A:4150:G:H5'    | 2.10                     | 0.52              |
| 1:1A:5053:U:H3'    | 1:1A:5054:C:C5     | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:54:A:H1'      | 13:2E:13:ARG:HG3   | 1.90                     | 0.52              |
| 5:1E:218:ASP:OD2   | 5:1E:348:ARG:NH1   | 2.43                     | 0.52              |
| 6:1F:152:LEU:HD23  | 6:1F:251:ILE:HG12  | 1.92                     | 0.52              |
| 6:1F:171:LEU:CD1   | 6:1F:177:TRP:HE3   | 2.15                     | 0.52              |
| 8:1H:147:GLY:HA3   | 8:1H:201:ILE:O     | 2.09                     | 0.52              |
| 14:2F:146:LEU:HD22 | 36:2b:122:LYS:CD   | 2.39                     | 0.52              |
| 26:2R:73:HIS:CE1   | 26:2R:115:LYS:HG2  | 2.44                     | 0.52              |
| 27:2S:118:ILE:O    | 27:2S:122:LYS:HG3  | 2.09                     | 0.52              |
| 37:2c:70:LEU:HB2   | 37:2c:87:ARG:NH1   | 2.24                     | 0.52              |
| 47:2m:533:A:HO2'   | 47:2m:534:G:P      | 2.33                     | 0.52              |
| 47:2m:835:C:C2'    | 47:2m:837:A:H1'    | 2.36                     | 0.52              |
| 47:2m:1124:C:OP1   | 49:2o:151:ARG:HG2  | 2.10                     | 0.52              |
| 47:2m:1297:U:H2'   | 47:2m:1298:G:H3'   | 1.91                     | 0.52              |
| 47:2m:1402:A:C5'   | 62:2i:51:LYS:HE2   | 2.39                     | 0.52              |
| 47:2m:1805:G:O2'   | 47:2m:1806:A:H5'   | 2.09                     | 0.52              |
| 51:2q:159:THR:HB   | 51:2q:173:ILE:HG13 | 1.91                     | 0.52              |
| 57:2w:17:TYR:CD1   | 57:2w:112:ILE:HD11 | 2.44                     | 0.52              |
| 60:2z:25:LYS:HG3   | 60:2z:55:ARG:NH1   | 2.24                     | 0.52              |
| 73:3K:142:GLU:OE1  | 73:3K:142:GLU:HA   | 2.10                     | 0.52              |
| 1:1A:271:C:O2'     | 1:1A:272:U:H5'     | 2.10                     | 0.52              |
| 1:1A:307:A:N3      | 1:1A:310:G:O2'     | 2.39                     | 0.52              |
| 1:1A:1301:C:H5''   | 1:1A:1302:U:OP2    | 2.09                     | 0.52              |
| 1:1A:2102:G:N2     | 1:1A:2104:G:N7     | 2.52                     | 0.52              |
| 1:1A:4098:A:N6     | 1:1A:4099:G:H21    | 2.05                     | 0.52              |
| 1:1A:4122:G:N7     | 35:2a:97:ILE:HD12  | 2.24                     | 0.52              |
| 1:1A:4233:A:OP1    | 43:2i:97:LYS:HA    | 2.10                     | 0.52              |
| 1:1A:4524:G:C2     | 5:1E:252:ALA:HB1   | 2.45                     | 0.52              |
| 3:1C:92:U:C2'      | 3:1C:93:C:H5'      | 2.40                     | 0.52              |
| 5:1E:302:ASN:HB3   | 5:1E:313:SER:HA    | 1.91                     | 0.52              |
| 6:1F:252:TRP:CH2   | 6:1F:260:LEU:HD11  | 2.44                     | 0.52              |
| 9:2A:144:TYR:HE2   | 9:2A:237:GLU:HG3   | 1.74                     | 0.52              |
| 12:2D:86:HIS:HB3   | 12:2D:139:ARG:HG2  | 1.90                     | 0.52              |
| 25:2Q:97:LYS:CG    | 25:2Q:98:PRO:HD3   | 2.32                     | 0.52              |
| 31:2W:37:MET:HE3   | 31:2W:37:MET:CA    | 2.29                     | 0.52              |
| 46:2l:95:LYS:HD3   | 46:2l:127:GLY:HA3  | 1.92                     | 0.52              |
| 47:2m:536:A:H8     | 47:2m:537:C:H1'    | 1.74                     | 0.52              |
| 47:2m:957:A:C2'    | 47:2m:958:G:H21    | 2.16                     | 0.52              |
| 47:2m:1482:C:H2'   | 47:2m:1483:A:O4'   | 2.09                     | 0.52              |
| 50:2p:37:VAL:CG1   | 50:2p:50:ILE:HD13  | 2.38                     | 0.52              |
| 52:2r:56:TYR:HA    | 52:2r:62:ARG:HG2   | 1.92                     | 0.52              |
| 53:2s:21:SER:O     | 53:2s:25:GLN:HG3   | 2.09                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:20:4:VAL:HG21  | 61:20:139:ALA:CB   | 2.40                     | 0.52              |
| 70:3H:50:VAL:HG23 | 70:3H:112:VAL:O    | 2.10                     | 0.52              |
| 70:3H:63:MET:CE   | 70:3H:98:ARG:HB3   | 2.39                     | 0.52              |
| 75:3M:23:ARG:HG2  | 78:3P:3:LEU:O      | 2.09                     | 0.52              |
| 76:3N:10:ARG:HH12 | 76:3N:70:THR:CG2   | 2.22                     | 0.52              |
| 1:1A:409:G:H2'    | 81:1A:5105:84D:N   | 2.25                     | 0.52              |
| 1:1A:452:A:O3'    | 8:1H:224:LYS:NZ    | 2.43                     | 0.52              |
| 1:1A:500:G:H4'    | 1:1A:504:G:P       | 2.49                     | 0.52              |
| 1:1A:1173:G:O2'   | 1:1A:1174:G:OP1    | 2.23                     | 0.52              |
| 1:1A:1199:G:H2'   | 1:1A:1200:G:H8     | 1.69                     | 0.52              |
| 1:1A:1327:C:H2'   | 1:1A:1328:G:C8     | 2.44                     | 0.52              |
| 1:1A:1617:G:H1'   | 1:1A:2513:A:H61    | 1.73                     | 0.52              |
| 1:1A:1886:G:C2'   | 1:1A:1887:G:H5'    | 2.40                     | 0.52              |
| 1:1A:3871:A:H2'   | 1:1A:3872:A:H8     | 1.72                     | 0.52              |
| 1:1A:4186:A:H2'   | 1:1A:4187:G:C8     | 2.45                     | 0.52              |
| 1:1A:4899:G:H3'   | 1:1A:4901:G:OP2    | 2.10                     | 0.52              |
| 1:1A:5003:U:H2'   | 1:1A:5004:C:H6     | 1.73                     | 0.52              |
| 2:1B:31:G:C2'     | 2:1B:32:A:H5'      | 2.39                     | 0.52              |
| 3:1C:16:G:O2'     | 3:1C:17:A:O5'      | 2.14                     | 0.52              |
| 3:1C:148:A:H2'    | 3:1C:149:G:C8      | 2.44                     | 0.52              |
| 5:1E:288:GLY:HA3  | 5:1E:330:PHE:CZ    | 2.45                     | 0.52              |
| 16:2H:178:HIS:HA  | 16:2H:181:HIS:NE2  | 2.25                     | 0.52              |
| 20:2L:77:GLY:O    | 20:2L:81:ARG:NH2   | 2.41                     | 0.52              |
| 20:2L:178:GLN:CA  | 20:2L:181:LYS:HE3  | 2.34                     | 0.52              |
| 32:2X:59:THR:HB   | 32:2X:60:PRO:CD    | 2.38                     | 0.52              |
| 38:2d:39:TYR:HB3  | 38:2d:40:PRO:HD3   | 1.91                     | 0.52              |
| 47:2m:837:A:H61   | 76:3N:9:THR:CG2    | 2.21                     | 0.52              |
| 47:2m:1004:U:H2'  | 47:2m:1005:G:C8    | 2.43                     | 0.52              |
| 47:2m:1241:A:O3'  | 47:2m:1242:U:H4'   | 2.09                     | 0.52              |
| 47:2m:1801:A:H2'  | 47:2m:1802:C:C6    | 2.45                     | 0.52              |
| 48:2n:50:ASN:HB3  | 48:2n:53:ARG:HG2   | 1.92                     | 0.52              |
| 49:2o:171:ILE:HB  | 49:2o:197:ILE:CD1  | 2.38                     | 0.52              |
| 50:2p:55:THR:O    | 50:2p:58:VAL:HG12  | 2.09                     | 0.52              |
| 50:2p:134:CYS:SG  | 50:2p:135:GLU:N    | 2.82                     | 0.52              |
| 53:2s:20:GLU:HA   | 53:2s:23:ILE:CD1   | 2.39                     | 0.52              |
| 56:2v:124:ASP:HB2 | 56:2v:146:THR:O    | 2.10                     | 0.52              |
| 59:2y:72:LYS:HG3  | 59:2y:73:LEU:HD22  | 1.91                     | 0.52              |
| 62:21:31:SER:HA   | 62:21:34:LYS:HG3   | 1.90                     | 0.52              |
| 69:3G:192:LEU:C   | 69:3G:192:LEU:HD23 | 2.34                     | 0.52              |
| 70:3H:140:ARG:HA  | 70:3H:143:LYS:HD3  | 1.92                     | 0.52              |
| 76:3N:94:HIS:HE2  | 76:3N:96:LEU:HD12  | 1.75                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:313:U:C2'    | 1:1A:314:G:H5'     | 2.40                     | 0.52              |
| 1:1A:513:U:H2'    | 1:1A:515:C:H5      | 1.75                     | 0.52              |
| 1:1A:1081:C:C2'   | 1:1A:1082:C:H5'    | 2.40                     | 0.52              |
| 1:1A:1243:C:H2'   | 1:1A:1244:G:O4'    | 2.09                     | 0.52              |
| 1:1A:1727:U:H2'   | 1:1A:1728:U:C6     | 2.44                     | 0.52              |
| 1:1A:1733:G:N3    | 1:1A:4214:A:H2'    | 2.25                     | 0.52              |
| 1:1A:1788:A:H2'   | 12:2D:22:PHE:CZ    | 2.44                     | 0.52              |
| 1:1A:2412:A:H2'   | 1:1A:2413:U:H6     | 1.73                     | 0.52              |
| 1:1A:2421:G:OP2   | 1:1A:2828:U:H1'    | 2.10                     | 0.52              |
| 1:1A:2639:U:O2    | 35:2a:26:PRO:HB3   | 2.09                     | 0.52              |
| 1:1A:3664:G:H2'   | 1:1A:3665:G:C8     | 2.42                     | 0.52              |
| 1:1A:3773:U:H5''  | 1:1A:3775:A:OP2    | 2.09                     | 0.52              |
| 1:1A:4108:G:H5'   | 1:1A:4109:G:OP2    | 2.10                     | 0.52              |
| 1:1A:4174:U:H2'   | 1:1A:4175:G:C8     | 2.44                     | 0.52              |
| 1:1A:4539:U:O2'   | 1:1A:4540:C:H5'    | 2.09                     | 0.52              |
| 2:1B:52:C:H4'     | 13:2E:11:PRO:CB    | 2.36                     | 0.52              |
| 4:1D:46:LYS:HG3   | 4:1D:62:VAL:HG23   | 1.92                     | 0.52              |
| 4:1D:95:GLN:HB3   | 44:2j:87:LYS:HZ1   | 1.75                     | 0.52              |
| 10:2B:108:GLN:O   | 10:2B:111:LYS:HG2  | 2.10                     | 0.52              |
| 46:2l:87:ILE:HA   | 46:2l:90:LEU:HB2   | 1.89                     | 0.52              |
| 47:2m:680:G:O2'   | 47:2m:681:U:H5'    | 2.10                     | 0.52              |
| 47:2m:816:A:H2'   | 47:2m:817:G:O4'    | 2.10                     | 0.52              |
| 47:2m:835:C:H2'   | 47:2m:837:A:C1'    | 2.38                     | 0.52              |
| 47:2m:1548:G:OP1  | 62:21:62:ARG:NH2   | 2.38                     | 0.52              |
| 47:2m:1754:G:H3'  | 47:2m:1755:C:H5''  | 1.92                     | 0.52              |
| 47:2m:1761:U:H2'  | 47:2m:1772:C:N4    | 2.24                     | 0.52              |
| 48:2n:116:PHE:HD1 | 48:2n:117:ARG:N    | 2.07                     | 0.52              |
| 52:2r:30:ILE:HB   | 52:2r:36:GLN:OE1   | 2.09                     | 0.52              |
| 52:2r:49:LEU:HD11 | 58:2x:49:TYR:HB2   | 1.92                     | 0.52              |
| 52:2r:129:GLY:HA3 | 52:2r:136:ARG:CZ   | 2.39                     | 0.52              |
| 57:2w:49:LEU:HD23 | 57:2w:53:GLN:HB3   | 1.90                     | 0.52              |
| 61:20:13:GLU:OE1  | 61:20:16:ARG:NH1   | 2.37                     | 0.52              |
| 62:21:51:LYS:HB3  | 62:21:90:ASP:O     | 2.10                     | 0.52              |
| 62:21:67:LYS:O    | 62:21:67:LYS:HG2   | 2.08                     | 0.52              |
| 64:3B:109:GLY:O   | 64:3B:119:ARG:HD3  | 2.10                     | 0.52              |
| 68:3F:11:LEU:HB3  | 68:3F:43:TRP:CZ3   | 2.44                     | 0.52              |
| 68:3F:156:PHE:CD1 | 68:3F:165:ILE:HG23 | 2.44                     | 0.52              |
| 72:3J:40:LYS:O    | 72:3J:44:LYS:HG2   | 2.09                     | 0.52              |
| 73:3K:5:HIS:HD2   | 73:3K:121:ARG:HG3  | 1.74                     | 0.52              |
| 1:1A:325:U:H2'    | 1:1A:326:C:H6      | 1.75                     | 0.52              |
| 1:1A:406:C:O2'    | 1:1A:407:A:P       | 2.67                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1212:G:O2'    | 1:1A:1213:G:H5'    | 2.09                     | 0.52              |
| 1:1A:1748:U:HO2'   | 1:1A:1749:A:H5'    | 1.73                     | 0.52              |
| 1:1A:3727:A:H8     | 1:1A:3727:A:OP2    | 1.93                     | 0.52              |
| 1:1A:3762:U:H2'    | 1:1A:3763:A:H8     | 1.72                     | 0.52              |
| 1:1A:4070:U:O2'    | 1:1A:4071:U:H5'    | 2.10                     | 0.52              |
| 1:1A:4265:U:H4'    | 1:1A:4266:G:O4'    | 2.09                     | 0.52              |
| 1:1A:4458:C:H2'    | 1:1A:4459:U:H6     | 1.74                     | 0.52              |
| 1:1A:4622:A:O2'    | 1:1A:4623:G:H5'    | 2.09                     | 0.52              |
| 1:1A:4881:U:O2'    | 1:1A:4882:U:H6     | 1.92                     | 0.52              |
| 7:1G:216:GLU:O     | 7:1G:220:LYS:HG2   | 2.10                     | 0.52              |
| 10:2B:80:ILE:CD1   | 16:2H:18:VAL:HG13  | 2.40                     | 0.52              |
| 13:2E:94:LEU:O     | 13:2E:174:ILE:HA   | 2.10                     | 0.52              |
| 16:2H:16:SER:HB2   | 37:2c:48:CYS:HB2   | 1.91                     | 0.52              |
| 47:2m:191:A:N6     | 47:2m:208:G:HO2'   | 2.06                     | 0.52              |
| 47:2m:303:C:O2     | 54:2t:184:ARG:NH1  | 2.43                     | 0.52              |
| 47:2m:438:G:N3     | 47:2m:438:G:H5''   | 2.25                     | 0.52              |
| 47:2m:605:A:N3     | 47:2m:639:C:H1'    | 2.24                     | 0.52              |
| 47:2m:1093:A:H2'   | 47:2m:1094:C:C6    | 2.45                     | 0.52              |
| 47:2m:1292:C:O2    | 47:2m:1295:A:N6    | 2.42                     | 0.52              |
| 47:2m:1612:G:H1'   | 60:2z:87:GLN:OE1   | 2.10                     | 0.52              |
| 47:2m:1622:U:O4    | 57:2w:122:THR:HG23 | 2.10                     | 0.52              |
| 49:2o:171:ILE:HD12 | 49:2o:197:ILE:HD13 | 1.92                     | 0.52              |
| 50:2p:29:LEU:CD2   | 50:2p:58:VAL:HG23  | 2.39                     | 0.52              |
| 50:2p:192:TRP:CE2  | 50:2p:203:PRO:HB3  | 2.45                     | 0.52              |
| 53:2s:43:LEU:HB2   | 53:2s:72:PHE:CE1   | 2.44                     | 0.52              |
| 56:2v:88:ILE:HD11  | 56:2v:109:MET:HE3  | 1.92                     | 0.52              |
| 57:2w:100:LYS:HG3  | 57:2w:101:THR:HG22 | 1.91                     | 0.52              |
| 60:2z:27:ALA:HA    | 60:2z:45:LEU:HD12  | 1.91                     | 0.52              |
| 60:2z:73:ASN:OD1   | 60:2z:73:ASN:O     | 2.27                     | 0.52              |
| 61:20:49:ASP:HB3   | 61:20:52:TRP:HB3   | 1.92                     | 0.52              |
| 62:21:48:LEU:HD13  | 62:21:93:SER:CB    | 2.40                     | 0.52              |
| 68:3F:152:SER:N    | 68:3F:168:CYS:O    | 2.43                     | 0.52              |
| 69:3G:121:ARG:NH1  | 69:3G:123:ARG:HG3  | 2.25                     | 0.52              |
| 74:3L:140:THR:O    | 74:3L:140:THR:HG22 | 2.08                     | 0.52              |
| 1:1A:137:G:H2'     | 1:1A:138:G:H8      | 1.69                     | 0.52              |
| 1:1A:266:C:H1'     | 1:1A:267:G:C8      | 2.44                     | 0.52              |
| 1:1A:485:C:OP2     | 1:1A:486:C:H5''    | 2.09                     | 0.52              |
| 1:1A:1907:A:C5'    | 9:2A:220:MET:HE3   | 2.39                     | 0.52              |
| 1:1A:2250:C:O2'    | 1:1A:2251:G:H5'    | 2.10                     | 0.52              |
| 1:1A:2355:G:O2'    | 1:1A:2356:U:H5'    | 2.09                     | 0.52              |
| 1:1A:2489:C:H4'    | 1:1A:2491:C:C4     | 2.45                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4230:C:O2'    | 1:1A:4231:C:H5'    | 2.09                     | 0.52              |
| 7:1G:243:ALA:O     | 7:1G:247:ILE:HD12  | 2.09                     | 0.52              |
| 15:2G:130:LEU:HD23 | 17:2I:177:LEU:HD22 | 1.91                     | 0.52              |
| 17:2I:186:GLU:HA   | 17:2I:189:ILE:HG12 | 1.91                     | 0.52              |
| 19:2K:177:ALA:HB1  | 29:2U:54:GLY:HA3   | 1.90                     | 0.52              |
| 23:2O:38:ASN:HA    | 23:2O:41:GLN:NE2   | 2.24                     | 0.52              |
| 23:2O:63:ILE:HA    | 23:2O:71:THR:O     | 2.09                     | 0.52              |
| 46:2I:143:ASN:H    | 46:2I:148:VAL:HG11 | 1.73                     | 0.52              |
| 46:2I:172:VAL:HG11 | 46:2I:179:LEU:CD1  | 2.40                     | 0.52              |
| 47:2m:71:G:C2      | 70:3H:170:ARG:HD3  | 2.45                     | 0.52              |
| 47:2m:1121:G:C2    | 47:2m:1122:A:C8    | 2.97                     | 0.52              |
| 47:2m:1301:A:H3'   | 47:2m:1301:A:N3    | 2.25                     | 0.52              |
| 47:2m:1488:C:O2'   | 47:2m:1490:G:H8    | 1.93                     | 0.52              |
| 49:2o:34:LYS:O     | 49:2o:232:HIS:HE1  | 1.92                     | 0.52              |
| 49:2o:73:ASP:OD1   | 74:3L:128:ARG:NH2  | 2.38                     | 0.52              |
| 50:2p:156:LEU:HD12 | 50:2p:157:MET:H    | 1.73                     | 0.52              |
| 52:2r:50:PRO:HG2   | 52:2r:90:VAL:HG22  | 1.90                     | 0.52              |
| 54:2t:56:ARG:CA    | 54:2t:180:GLY:HA2  | 2.39                     | 0.52              |
| 54:2t:62:VAL:HG13  | 54:2t:76:THR:O     | 2.10                     | 0.52              |
| 58:2x:15:ARG:HA    | 58:2x:19:ALA:O     | 2.09                     | 0.52              |
| 58:2x:50:LYS:C     | 58:2x:53:GLU:HG3   | 2.35                     | 0.52              |
| 58:2x:139:ALA:O    | 58:2x:140:ARG:HD3  | 2.10                     | 0.52              |
| 62:2I:22:ILE:HD13  | 62:2I:114:VAL:HA   | 1.91                     | 0.52              |
| 62:2I:104:ILE:HG23 | 62:2I:105:SER:H    | 1.75                     | 0.52              |
| 65:3C:47:ALA:HA    | 65:3C:50:VAL:HG21  | 1.91                     | 0.52              |
| 68:3F:108:VAL:HA   | 68:3F:124:SER:HA   | 1.91                     | 0.52              |
| 68:3F:168:CYS:CB   | 68:3F:195:LEU:HD13 | 2.38                     | 0.52              |
| 71:3I:115:PHE:HE1  | 71:3I:122:SER:N    | 2.08                     | 0.52              |
| 75:3M:53:ILE:HD13  | 78:3P:24:LEU:CG    | 2.36                     | 0.52              |
| 77:3O:47:LEU:HD22  | 77:3O:79:ILE:HA    | 1.92                     | 0.52              |
| 1:1A:222:C:H2'     | 1:1A:223:G:O4'     | 2.09                     | 0.52              |
| 1:1A:302:C:OP1     | 16:2H:68:ARG:HB2   | 2.09                     | 0.52              |
| 1:1A:368:C:O4'     | 6:1F:83:GLY:HA3    | 2.08                     | 0.52              |
| 1:1A:1269:G:O2'    | 1:1A:1440:U:H4'    | 2.10                     | 0.52              |
| 1:1A:1727:U:H2'    | 1:1A:1728:U:H6     | 1.75                     | 0.52              |
| 1:1A:1762:C:H3'    | 1:1A:1763:C:C5'    | 2.36                     | 0.52              |
| 1:1A:2434:G:O2'    | 1:1A:2527:A:N1     | 2.42                     | 0.52              |
| 1:1A:2530:U:OP1    | 1:1A:2531:C:H5     | 1.93                     | 0.52              |
| 1:1A:2733:C:O2'    | 1:1A:2734:U:H5'    | 2.10                     | 0.52              |
| 1:1A:3917:A:H2'    | 1:1A:3918:G:H8     | 1.75                     | 0.52              |
| 1:1A:3937:C:H1'    | 16:2H:125:SER:CB   | 2.40                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:5026:U:H4'   | 1:1A:5027:C:H5'    | 1.91                     | 0.52              |
| 7:1G:121:GLY:HA3  | 7:1G:168:ASP:O     | 2.09                     | 0.52              |
| 11:2C:118:LEU:CD1 | 11:2C:167:VAL:HG22 | 2.34                     | 0.52              |
| 33:2Y:84:GLU:OE2  | 45:2k:20:ARG:NH1   | 2.41                     | 0.52              |
| 47:2m:482:G:OP1   | 64:3B:76:LYS:HA    | 2.10                     | 0.52              |
| 47:2m:495:U:H2'   | 47:2m:496:C:O4'    | 2.10                     | 0.52              |
| 47:2m:1129:G:H2'  | 47:2m:1130:G:N9    | 2.25                     | 0.52              |
| 47:2m:1610:G:H2'  | 47:2m:1611:G:O4'   | 2.10                     | 0.52              |
| 47:2m:1673:U:H2'  | 47:2m:1674:G:O4'   | 2.10                     | 0.52              |
| 49:2o:36:PRO:HD3  | 49:2o:98:THR:CG2   | 2.40                     | 0.52              |
| 50:2p:76:ARG:HB2  | 55:2u:22:VAL:HG21  | 1.91                     | 0.52              |
| 52:2r:92:ILE:CD1  | 52:2r:169:ILE:HG23 | 2.39                     | 0.52              |
| 52:2r:165:ASN:OD1 | 52:2r:166:ILE:N    | 2.42                     | 0.52              |
| 58:2x:21:ALA:HB2  | 58:2x:72:VAL:CG1   | 2.35                     | 0.52              |
| 60:2z:105:ASN:HA  | 60:2z:108:ARG:HG2  | 1.91                     | 0.52              |
| 62:21:66:ARG:O    | 62:21:67:LYS:HB3   | 2.10                     | 0.52              |
| 63:3A:9:VAL:O     | 63:3A:9:VAL:CG2    | 2.58                     | 0.52              |
| 68:3F:5:MET:HE3   | 68:3F:312:VAL:HG12 | 1.91                     | 0.52              |
| 73:3K:62:GLN:O    | 73:3K:66:VAL:HG12  | 2.10                     | 0.52              |
| 75:3M:62:VAL:HG11 | 78:3P:8:LEU:HD23   | 1.91                     | 0.52              |
| 76:3N:60:PHE:CE1  | 76:3N:71:GLY:HA3   | 2.45                     | 0.52              |
| 1:1A:25:A:H2'     | 1:1A:26:C:H6       | 1.75                     | 0.52              |
| 1:1A:248:C:N3     | 1:1A:249:C:C5      | 2.77                     | 0.52              |
| 1:1A:493:G:H2'    | 1:1A:494:U:C5'     | 2.37                     | 0.52              |
| 1:1A:1551:C:H2'   | 1:1A:1552:G:O4'    | 2.10                     | 0.52              |
| 1:1A:2711:G:H3'   | 1:1A:2712:G:H5''   | 1.91                     | 0.52              |
| 1:1A:4080:C:H2'   | 1:1A:4081:G:H8     | 1.74                     | 0.52              |
| 1:1A:4091:G:O2'   | 1:1A:4092:G:H5'    | 2.10                     | 0.52              |
| 4:1D:117:GLU:OE2  | 4:1D:163:ARG:NH2   | 2.42                     | 0.52              |
| 7:1G:110:LEU:HD23 | 7:1G:115:MET:HE3   | 1.92                     | 0.52              |
| 8:1H:202:ASP:C    | 8:1H:203:ILE:HD13  | 2.35                     | 0.52              |
| 15:2G:33:GLN:HB3  | 21:2M:145:PHE:HZ   | 1.74                     | 0.52              |
| 23:2O:39:PHE:CE2  | 23:2O:43:LEU:HD21  | 2.45                     | 0.52              |
| 25:2Q:45:ASN:ND2  | 25:2Q:46:PRO:HD2   | 2.25                     | 0.52              |
| 26:2R:111:GLN:OE1 | 26:2R:111:GLN:HA   | 2.10                     | 0.52              |
| 46:2l:176:ASP:O   | 46:2l:180:VAL:HG22 | 2.10                     | 0.52              |
| 47:2m:383:G:O2'   | 56:2v:133:PRO:O    | 2.28                     | 0.52              |
| 47:2m:502:C:H3'   | 47:2m:503:C:C5     | 2.45                     | 0.52              |
| 47:2m:537:C:H3'   | 47:2m:538:U:H5'    | 1.92                     | 0.52              |
| 47:2m:993:G:OP1   | 47:2m:1131:G:N2    | 2.24                     | 0.52              |
| 47:2m:1286:G:H22  | 72:3J:33:ARG:HG3   | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1499:U:H4'   | 50:2p:176:LEU:HD13 | 1.92                     | 0.52              |
| 47:2m:1643:U:O2'   | 47:2m:1644:C:H6    | 1.90                     | 0.52              |
| 49:2o:212:VAL:HG12 | 49:2o:212:VAL:O    | 2.09                     | 0.52              |
| 50:2p:68:GLU:HG3   | 55:2u:70:TYR:CE2   | 2.45                     | 0.52              |
| 50:2p:69:LEU:HD23  | 50:2p:73:VAL:HG23  | 1.92                     | 0.52              |
| 52:2r:17:ILE:HD13  | 52:2r:46:ALA:CB    | 2.40                     | 0.52              |
| 55:2u:13:GLU:HG3   | 55:2u:14:LEU:N     | 2.25                     | 0.52              |
| 57:2w:57:LEU:HG    | 57:2w:89:MET:HE2   | 1.92                     | 0.52              |
| 58:2x:8:GLN:HA     | 58:2x:99:TYR:CZ    | 2.45                     | 0.52              |
| 60:2z:28:PHE:CZ    | 61:20:45:LEU:HD21  | 2.44                     | 0.52              |
| 62:21:38:ASP:HA    | 62:21:41:ARG:CD    | 2.28                     | 0.52              |
| 68:3F:52:TYR:HE2   | 68:3F:309:VAL:HG11 | 1.75                     | 0.52              |
| 68:3F:76:GLN:O     | 68:3F:92:LEU:HD23  | 2.10                     | 0.52              |
| 68:3F:291:TRP:HA   | 68:3F:298:LEU:HD23 | 1.92                     | 0.52              |
| 69:3G:241:PHE:O    | 69:3G:244:ILE:HG12 | 2.10                     | 0.52              |
| 70:3H:63:MET:SD    | 70:3H:98:ARG:HB3   | 2.49                     | 0.52              |
| 77:3O:46:ASN:N     | 77:3O:46:ASN:OD1   | 2.42                     | 0.52              |
| 1:1A:123:C:H2'     | 1:1A:124:C:H6      | 1.75                     | 0.51              |
| 1:1A:483:G:O6      | 1:1A:485:C:H4'     | 2.09                     | 0.51              |
| 1:1A:518:G:H1      | 1:1A:643:C:C2'     | 2.23                     | 0.51              |
| 1:1A:518:G:H1      | 1:1A:643:C:H2'     | 1.75                     | 0.51              |
| 1:1A:1179:U:H5'    | 1:1A:1180:C:H5''   | 1.92                     | 0.51              |
| 1:1A:1510:G:H2'    | 1:1A:1511:U:C6     | 2.45                     | 0.51              |
| 1:1A:2257:C:O2     | 1:1A:2257:C:C2'    | 2.58                     | 0.51              |
| 1:1A:2847:G:O2'    | 1:1A:2848:G:H5'    | 2.10                     | 0.51              |
| 1:1A:3928:A:OP1    | 16:2H:90:ASN:ND2   | 2.41                     | 0.51              |
| 1:1A:4862:G:H3'    | 1:1A:4862:G:N3     | 2.25                     | 0.51              |
| 1:1A:4988:U:C5     | 1:1A:5060:A:H2'    | 2.46                     | 0.51              |
| 1:1A:4991:U:O2'    | 1:1A:4992:G:H5'    | 2.10                     | 0.51              |
| 2:1B:13:A:H5'      | 2:1B:110:G:OP1     | 2.10                     | 0.51              |
| 4:1D:14:SER:H      | 4:1D:17:ARG:HG3    | 1.75                     | 0.51              |
| 9:2A:150:VAL:O     | 9:2A:154:ILE:HG12  | 2.10                     | 0.51              |
| 12:2D:46:PHE:CE1   | 12:2D:141:LYS:HD2  | 2.46                     | 0.51              |
| 15:2G:36:ALA:HB2   | 15:2G:52:PHE:CE1   | 2.45                     | 0.51              |
| 21:2M:69:GLU:OE1   | 21:2M:102:THR:HG22 | 2.11                     | 0.51              |
| 25:2Q:76:VAL:HG12  | 25:2Q:77:LYS:H     | 1.74                     | 0.51              |
| 26:2R:112:ALA:O    | 26:2R:116:LEU:HG   | 2.10                     | 0.51              |
| 28:2T:36:ARG:HD2   | 28:2T:40:HIS:CD2   | 2.45                     | 0.51              |
| 33:2Y:62:SER:OG    | 33:2Y:67:LYS:HG3   | 2.11                     | 0.51              |
| 33:2Y:128:ARG:O    | 33:2Y:129:LEU:HD23 | 2.09                     | 0.51              |
| 46:2L:94:ASN:ND2   | 46:2L:95:LYS:H     | 2.08                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:188:C:H3'   | 47:2m:189:U:C6     | 2.45                     | 0.51              |
| 47:2m:291:G:H1'   | 47:2m:292:A:H2'    | 1.92                     | 0.51              |
| 47:2m:1281:G:O2'  | 47:2m:1282:A:P     | 2.68                     | 0.51              |
| 47:2m:1283:C:H5'  | 47:2m:1284:A:P     | 2.50                     | 0.51              |
| 47:2m:1511:U:O2'  | 47:2m:1512:C:H6    | 1.93                     | 0.51              |
| 47:2m:1539:U:H2'  | 47:2m:1540:G:C8    | 2.45                     | 0.51              |
| 47:2m:1794:C:H2'  | 47:2m:1795:G:H8    | 1.74                     | 0.51              |
| 48:2n:142:LEU:HG  | 48:2n:142:LEU:O    | 2.09                     | 0.51              |
| 50:2p:70:THR:HG22 | 50:2p:86:LEU:CG    | 2.40                     | 0.51              |
| 51:2q:29:PRO:HG2  | 51:2q:46:ILE:CG2   | 2.40                     | 0.51              |
| 51:2q:106:LYS:HD2 | 51:2q:108:ARG:HH22 | 1.74                     | 0.51              |
| 52:2r:40:ALA:HA   | 52:2r:45:TYR:OH    | 2.11                     | 0.51              |
| 52:2r:60:ARG:O    | 52:2r:61:PHE:HB2   | 2.11                     | 0.51              |
| 52:2r:79:HIS:CG   | 52:2r:159:ARG:HD3  | 2.44                     | 0.51              |
| 55:2u:27:VAL:HB   | 67:3E:7:TYR:OH     | 2.10                     | 0.51              |
| 56:2v:90:ARG:HG2  | 56:2v:107:LYS:O    | 2.10                     | 0.51              |
| 56:2v:150:GLY:HA2 | 56:2v:153:LYS:HZ2  | 1.75                     | 0.51              |
| 58:2x:31:LEU:HB3  | 58:2x:67:ASP:HB3   | 1.92                     | 0.51              |
| 59:2y:24:LEU:HD13 | 59:2y:31:ASN:ND2   | 2.24                     | 0.51              |
| 59:2y:60:ARG:HG3  | 59:2y:63:ARG:NH2   | 2.25                     | 0.51              |
| 62:21:17:ILE:N    | 62:21:94:PRO:HG3   | 2.25                     | 0.51              |
| 65:3C:62:TYR:OH   | 74:3L:128:ARG:HA   | 2.10                     | 0.51              |
| 65:3C:87:ARG:HG2  | 65:3C:91:ALA:HB3   | 1.91                     | 0.51              |
| 68:3F:32:LEU:HD13 | 68:3F:40:ILE:HG22  | 1.92                     | 0.51              |
| 69:3G:278:THR:OG1 | 69:3G:280:VAL:HG13 | 2.10                     | 0.51              |
| 70:3H:23:LYS:HD3  | 70:3H:41:LEU:HB2   | 1.91                     | 0.51              |
| 70:3H:32:MET:HB3  | 70:3H:65:GLN:NE2   | 2.25                     | 0.51              |
| 70:3H:181:THR:OG1 | 70:3H:182:PRO:HD2  | 2.10                     | 0.51              |
| 1:1A:1855:G:H2'   | 1:1A:1856:C:C6     | 2.45                     | 0.51              |
| 1:1A:3775:A:H5'   | 1:1A:3776:G:OP2    | 2.10                     | 0.51              |
| 1:1A:4670:C:O3'   | 1:1A:4671:C:H3'    | 2.10                     | 0.51              |
| 1:1A:4749:C:H3'   | 1:1A:4750:G:H5''   | 1.91                     | 0.51              |
| 1:1A:4866:C:O2'   | 1:1A:4867:G:H5'    | 2.10                     | 0.51              |
| 1:1A:4889:G:O2'   | 1:1A:4890:G:H5'    | 2.10                     | 0.51              |
| 1:1A:5009:G:O2'   | 1:1A:5010:U:H5'    | 2.10                     | 0.51              |
| 13:2E:167:GLN:NE2 | 13:2E:174:ILE:HD12 | 2.25                     | 0.51              |
| 28:2T:33:THR:O    | 28:2T:34:SER:HB3   | 2.09                     | 0.51              |
| 43:2i:14:LYS:HD3  | 43:2i:79:SER:OG    | 2.09                     | 0.51              |
| 47:2m:837:A:H61   | 76:3N:9:THR:HB     | 1.75                     | 0.51              |
| 47:2m:926:A:H5''  | 73:3K:90:HIS:CD2   | 2.44                     | 0.51              |
| 47:2m:952:G:H21   | 74:3L:52:THR:HG1   | 1.57                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1089:G:H2'   | 47:2m:1090:C:C6    | 2.45                     | 0.51              |
| 47:2m:1208:A:O2'   | 47:2m:1209:A:H5'   | 2.09                     | 0.51              |
| 47:2m:1284:A:H62   | 72:3J:91:LEU:HD21  | 1.74                     | 0.51              |
| 47:2m:1447:G:O2'   | 47:2m:1448:A:H5'   | 2.10                     | 0.51              |
| 47:2m:1673:U:H5''  | 58:2x:78:VAL:CG2   | 2.40                     | 0.51              |
| 50:2p:5:ILE:HG23   | 50:2p:10:LYS:HD2   | 1.90                     | 0.51              |
| 50:2p:136:VAL:HG13 | 50:2p:186:VAL:HG22 | 1.93                     | 0.51              |
| 52:2r:41:VAL:HG22  | 52:2r:41:VAL:O     | 2.11                     | 0.51              |
| 56:2v:68:ILE:HG13  | 56:2v:143:LEU:HD21 | 1.92                     | 0.51              |
| 58:2x:108:ILE:HG13 | 58:2x:109:LYS:N    | 2.25                     | 0.51              |
| 60:2z:89:ASP:OD2   | 60:2z:106:LYS:NZ   | 2.23                     | 0.51              |
| 64:3B:49:GLY:HA3   | 64:3B:72:VAL:CG2   | 2.40                     | 0.51              |
| 64:3B:129:SER:O    | 64:3B:133:LEU:HG   | 2.10                     | 0.51              |
| 67:3E:30:LEU:O     | 67:3E:31:ILE:HD12  | 2.10                     | 0.51              |
| 1:1A:116:G:H2'     | 1:1A:117:C:C6      | 2.45                     | 0.51              |
| 1:1A:162:A:H2'     | 1:1A:163:A:C8      | 2.45                     | 0.51              |
| 1:1A:1236:C:O2'    | 1:1A:1237:C:H5'    | 2.11                     | 0.51              |
| 1:1A:1847:C:H2'    | 1:1A:1848:C:C6     | 2.46                     | 0.51              |
| 1:1A:2250:C:H2'    | 1:1A:2251:G:C8     | 2.44                     | 0.51              |
| 1:1A:2256:C:C2'    | 1:1A:2257:C:H6     | 2.23                     | 0.51              |
| 1:1A:3770:U:O2'    | 1:1A:3771:C:H5'    | 2.11                     | 0.51              |
| 1:1A:3870:C:H2'    | 1:1A:3871:A:C8     | 2.46                     | 0.51              |
| 1:1A:4063:U:H3'    | 1:1A:4064:C:H6     | 1.74                     | 0.51              |
| 1:1A:4684:A:H2'    | 1:1A:4685:U:O4'    | 2.09                     | 0.51              |
| 1:1A:5005:G:H22    | 1:1A:5041:G:H1'    | 1.75                     | 0.51              |
| 4:1D:130:SER:HA    | 4:1D:169:VAL:HG12  | 1.91                     | 0.51              |
| 8:1H:145:THR:O     | 8:1H:148:THR:HG22  | 2.11                     | 0.51              |
| 8:1H:147:GLY:HA2   | 8:1H:203:ILE:HG12  | 1.91                     | 0.51              |
| 11:2C:150:ASP:HB3  | 11:2C:153:LEU:HB2  | 1.92                     | 0.51              |
| 13:2E:175:LEU:CB   | 13:2E:176:PRO:HD2  | 2.38                     | 0.51              |
| 28:2T:123:LYS:C    | 28:2T:124:THR:HG23 | 2.36                     | 0.51              |
| 39:2e:24:LYS:HD3   | 39:2e:69:LEU:HD21  | 1.93                     | 0.51              |
| 46:2l:33:GLU:HA    | 46:2l:168:ALA:HA   | 1.92                     | 0.51              |
| 47:2m:188:C:H42    | 47:2m:212:C:N4     | 2.08                     | 0.51              |
| 47:2m:814:U:OP1    | 51:2q:22:LYS:NZ    | 2.43                     | 0.51              |
| 47:2m:929:G:H2'    | 47:2m:930:C:O4'    | 2.10                     | 0.51              |
| 47:2m:940:U:H2'    | 47:2m:941:C:C6     | 2.45                     | 0.51              |
| 47:2m:1235:G:O6    | 60:2z:137:LYS:HE3  | 2.10                     | 0.51              |
| 47:2m:1267:C:N3    | 47:2m:1516:G:N1    | 2.59                     | 0.51              |
| 47:2m:1453:C:H4'   | 59:2y:49:LYS:HG3   | 1.92                     | 0.51              |
| 47:2m:1552:G:H5''  | 47:2m:1556:A:C2    | 2.46                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:1563:G:OP1  | 61:20:121:ARG:NH1  | 2.43                     | 0.51              |
| 47:2m:1596:U:C2'  | 47:2m:1597:C:H5'   | 2.41                     | 0.51              |
| 47:2m:1776:G:H3'  | 47:2m:1776:G:N3    | 2.26                     | 0.51              |
| 49:2o:71:LEU:HG   | 49:2o:78:GLU:CB    | 2.41                     | 0.51              |
| 50:2p:61:GLU:HG3  | 50:2p:64:ARG:CB    | 2.40                     | 0.51              |
| 52:2r:48:TYR:HE2  | 58:2x:56:LEU:HD13  | 1.74                     | 0.51              |
| 52:2r:121:PRO:CB  | 52:2r:193:LYS:HG2  | 2.39                     | 0.51              |
| 60:2z:33:ILE:HG22 | 60:2z:36:VAL:HB    | 1.93                     | 0.51              |
| 60:2z:47:LYS:HE2  | 60:2z:77:TYR:HB3   | 1.91                     | 0.51              |
| 67:3E:13:LYS:O    | 67:3E:18:SER:OG    | 2.17                     | 0.51              |
| 68:3F:103:GLY:HA3 | 68:3F:132:TRP:HZ2  | 1.75                     | 0.51              |
| 68:3F:106:LYS:CE  | 68:3F:125:ARG:HB3  | 2.40                     | 0.51              |
| 68:3F:313:THR:O   | 68:3F:314:ILE:HG22 | 2.10                     | 0.51              |
| 73:3K:98:VAL:O    | 73:3K:102:LEU:HD23 | 2.09                     | 0.51              |
| 76:3N:35:VAL:HG13 | 76:3N:40:ILE:CD1   | 2.40                     | 0.51              |
| 1:1A:694:C:O2'    | 1:1A:695:G:H5'     | 2.11                     | 0.51              |
| 1:1A:1528:U:H2'   | 1:1A:1529:G:H8     | 1.74                     | 0.51              |
| 1:1A:3635:A:C2'   | 1:1A:3636:C:H5'    | 2.39                     | 0.51              |
| 1:1A:3945:A:C3'   | 1:1A:3946:G:H5''   | 2.41                     | 0.51              |
| 1:1A:4071:U:H2'   | 1:1A:4072:C:C6     | 2.46                     | 0.51              |
| 1:1A:4349:C:H3'   | 1:1A:4350:C:H5'    | 1.92                     | 0.51              |
| 1:1A:4424:A:C4    | 1:1A:4425:G:C8     | 2.99                     | 0.51              |
| 28:2T:14:LEU:HB3  | 35:2a:88:ARG:HG3   | 1.91                     | 0.51              |
| 46:2l:25:ARG:HD3  | 46:2l:210:MET:HE1  | 1.91                     | 0.51              |
| 46:2l:71:GLN:H    | 46:2l:84:HIS:CE1   | 2.28                     | 0.51              |
| 47:2m:71:G:C3'    | 47:2m:72:C:H5''    | 2.36                     | 0.51              |
| 47:2m:188:C:H2'   | 47:2m:189:U:O4'    | 2.11                     | 0.51              |
| 47:2m:820:U:P     | 71:3I:79:ARG:HH22  | 2.34                     | 0.51              |
| 47:2m:972:A:H2'   | 47:2m:972:A:N3     | 2.25                     | 0.51              |
| 47:2m:1198:G:H2'  | 47:2m:1199:A:H8    | 1.74                     | 0.51              |
| 47:2m:1540:G:OP1  | 61:20:39:LEU:HD13  | 2.11                     | 0.51              |
| 47:2m:1543:U:O2'  | 47:2m:1544:C:OP2   | 2.24                     | 0.51              |
| 49:2o:30:TRP:CG   | 74:3L:19:PRO:HB3   | 2.45                     | 0.51              |
| 52:2r:35:LEU:CD2  | 52:2r:147:VAL:HG22 | 2.40                     | 0.51              |
| 62:21:41:ARG:HG2  | 62:21:42:GLY:N     | 2.25                     | 0.51              |
| 68:3F:253:GLY:HA2 | 68:3F:285:GLN:OE1  | 2.11                     | 0.51              |
| 71:3I:28:GLU:HG3  | 71:3I:40:LYS:CD    | 2.40                     | 0.51              |
| 1:1A:226:G:N7     | 6:1F:184:TYR:OH    | 2.37                     | 0.51              |
| 1:1A:667:A:C5'    | 1:1A:668:C:H5''    | 2.32                     | 0.51              |
| 1:1A:1457:G:O2'   | 1:1A:1458:C:H5'    | 2.10                     | 0.51              |
| 1:1A:1961:G:N2    | 1:1A:2024:G:O2'    | 2.31                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:2389:A:H2'    | 1:1A:2390:G:C8    | 2.46                     | 0.51              |
| 1:1A:2521:G:H5'    | 1:1A:2640:G:H1'   | 1.92                     | 0.51              |
| 1:1A:2521:G:H2'    | 1:1A:2522:G:H8    | 1.74                     | 0.51              |
| 1:1A:2528:G:H21    | 1:1A:2529:A:C5'   | 2.24                     | 0.51              |
| 1:1A:3604:A:H4'    | 1:1A:3604:A:OP1   | 2.11                     | 0.51              |
| 1:1A:3938:G:OP2    | 16:2H:24:ARG:NH2  | 2.27                     | 0.51              |
| 1:1A:3974:G:H2'    | 1:1A:3975:C:C5'   | 2.31                     | 0.51              |
| 1:1A:3974:G:H21    | 1:1A:4051:C:H5'   | 1.74                     | 0.51              |
| 1:1A:4053:A:H3'    | 1:1A:4053:A:N3    | 2.25                     | 0.51              |
| 1:1A:4708:A:C2     | 1:1A:4709:U:H5'   | 2.44                     | 0.51              |
| 3:1C:33:G:H5''     | 3:1C:34:U:OP1     | 2.10                     | 0.51              |
| 3:1C:47:C:H1'      | 3:1C:61:A:H2'     | 1.93                     | 0.51              |
| 7:1G:62:CYS:HB3    | 7:1G:105:LEU:HD22 | 1.93                     | 0.51              |
| 11:2C:51:LYS:HG2   | 11:2C:52:LYS:HG2  | 1.92                     | 0.51              |
| 11:2C:95:VAL:HG22  | 41:2g:82:LEU:HD13 | 1.92                     | 0.51              |
| 12:2D:34:PHE:HA    | 12:2D:89:VAL:HG22 | 1.92                     | 0.51              |
| 24:2P:107:ASN:OD1  | 24:2P:111:GLU:HG2 | 2.11                     | 0.51              |
| 47:2m:643:A:H4'    | 47:2m:644:G:C5'   | 2.28                     | 0.51              |
| 47:2m:1324:G:O2'   | 47:2m:1325:G:H5'  | 2.11                     | 0.51              |
| 47:2m:1326:U:H1'   | 47:2m:1494:U:C6   | 2.45                     | 0.51              |
| 47:2m:1648:G:C8    | 58:2x:125:ARG:HB2 | 2.45                     | 0.51              |
| 48:2n:189:ILE:HG23 | 48:2n:193:HIS:NE2 | 2.24                     | 0.51              |
| 50:2p:5:ILE:HG21   | 50:2p:10:LYS:HD2  | 1.93                     | 0.51              |
| 51:2q:212:ASP:OD2  | 51:2q:216:ASN:ND2 | 2.42                     | 0.51              |
| 53:2s:158:LEU:HB2  | 53:2s:189:PHE:CE2 | 2.46                     | 0.51              |
| 61:20:125:PRO:HA   | 61:20:128:GLN:NE2 | 2.26                     | 0.51              |
| 62:21:55:ARG:HG2   | 62:21:87:ARG:NE   | 2.25                     | 0.51              |
| 68:3F:176:VAL:HG12 | 68:3F:186:THR:HB  | 1.92                     | 0.51              |
| 68:3F:254:PRO:CG   | 68:3F:283:PRO:HB2 | 2.41                     | 0.51              |
| 70:3H:139:SER:HA   | 70:3H:142:ARG:NE  | 2.25                     | 0.51              |
| 71:3I:33:GLY:HA3   | 79:3Q:38:TYR:CD1  | 2.45                     | 0.51              |
| 72:3J:31:LEU:HA    | 72:3J:112:LYS:CE  | 2.34                     | 0.51              |
| 77:3O:62:VAL:HA    | 77:3O:65:TYR:CZ   | 2.45                     | 0.51              |
| 1:1A:377:A:H2'     | 1:1A:378:A:O4'    | 2.11                     | 0.51              |
| 1:1A:444:G:H2'     | 1:1A:445:U:C6     | 2.46                     | 0.51              |
| 1:1A:968:C:O4'     | 8:1H:110:ARG:NH2  | 2.43                     | 0.51              |
| 1:1A:1197:C:O2'    | 1:1A:1198:G:OP1   | 2.20                     | 0.51              |
| 1:1A:2333:G:O2'    | 1:1A:2334:C:H5'   | 2.11                     | 0.51              |
| 1:1A:2810:U:H2'    | 1:1A:2811:G:O4'   | 2.10                     | 0.51              |
| 1:1A:3754:G:H2'    | 1:1A:3755:G:H8    | 1.75                     | 0.51              |
| 1:1A:3946:G:N2     | 1:1A:4067:U:O2    | 2.30                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:3969:G:H1'    | 46:2l:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:1A:4060:U:HO2'   | 1:1A:4061:G:P      | 2.34                     | 0.51              |
| 1:1A:4600:G:H1'    | 1:1A:4609:G:O6     | 2.10                     | 0.51              |
| 7:1G:277:LYS:O     | 7:1G:280:VAL:HG13  | 2.10                     | 0.51              |
| 9:2A:241:ASN:O     | 9:2A:245:ARG:HG2   | 2.09                     | 0.51              |
| 13:2E:96:LYS:CG    | 13:2E:163:MET:HE1  | 2.35                     | 0.51              |
| 17:2I:54:TYR:OH    | 17:2I:73:PHE:O     | 2.29                     | 0.51              |
| 18:2J:108:ASP:OD1  | 18:2J:111:SER:OG   | 2.26                     | 0.51              |
| 25:2Q:123:LYS:HE3  | 47:2m:322:C:H5''   | 1.92                     | 0.51              |
| 33:2Y:84:GLU:OE2   | 45:2k:20:ARG:NH2   | 2.41                     | 0.51              |
| 46:2l:31:THR:HG23  | 46:2l:171:HIS:CD2  | 2.46                     | 0.51              |
| 46:2l:107:TYR:O    | 46:2l:133:LYS:NZ   | 2.38                     | 0.51              |
| 47:2m:10:G:H1'     | 69:3G:115:GLN:HG2  | 1.93                     | 0.51              |
| 47:2m:186:C:H2'    | 47:2m:187:G:N7     | 2.26                     | 0.51              |
| 47:2m:222:U:H2'    | 47:2m:223:C:C6     | 2.46                     | 0.51              |
| 47:2m:600:G:O2'    | 47:2m:601:G:H5'    | 2.10                     | 0.51              |
| 47:2m:696:G:H2'    | 47:2m:697:G:H5''   | 1.91                     | 0.51              |
| 47:2m:1047:C:O2'   | 47:2m:1048:G:H5'   | 2.11                     | 0.51              |
| 47:2m:1302:G:H1'   | 80:3R:95:ARG:NH1   | 2.26                     | 0.51              |
| 47:2m:1462:U:H5''  | 47:2m:1464:C:H41   | 1.76                     | 0.51              |
| 47:2m:1539:U:OP1   | 61:20:43:LYS:HB2   | 2.11                     | 0.51              |
| 47:2m:1552:G:H2'   | 50:2p:3:VAL:CG1    | 2.31                     | 0.51              |
| 47:2m:1607:A:H2'   | 47:2m:1608:U:O4'   | 2.11                     | 0.51              |
| 47:2m:1864:U:H3'   | 65:3C:5:ARG:HH21   | 1.76                     | 0.51              |
| 48:2n:20:ALA:CB    | 59:2y:91:LEU:HA    | 2.40                     | 0.51              |
| 48:2n:24:HIS:CB    | 48:2n:51:LEU:HD21  | 2.41                     | 0.51              |
| 48:2n:85:ARG:HG3   | 48:2n:89:LYS:NZ    | 2.26                     | 0.51              |
| 50:2p:96:LEU:HD23  | 50:2p:198:ILE:HG23 | 1.93                     | 0.51              |
| 52:2r:126:THR:HG22 | 52:2r:139:VAL:HG11 | 1.91                     | 0.51              |
| 54:2t:121:LEU:HD12 | 54:2t:122:GLY:H    | 1.76                     | 0.51              |
| 54:2t:141:ARG:HG2  | 54:2t:145:ILE:CD1  | 2.39                     | 0.51              |
| 59:2y:107:LYS:NZ   | 59:2y:107:LYS:HB3  | 2.26                     | 0.51              |
| 60:2z:125:HIS:NE2  | 60:2z:131:VAL:HG11 | 2.26                     | 0.51              |
| 61:20:29:LYS:HD2   | 61:20:30:VAL:N     | 2.25                     | 0.51              |
| 61:20:76:THR:HB    | 61:20:94:ARG:HB2   | 1.92                     | 0.51              |
| 68:3F:152:SER:HB2  | 68:3F:168:CYS:C    | 2.35                     | 0.51              |
| 68:3F:159:ASN:ND2  | 68:3F:204:GLY:HA3  | 2.26                     | 0.51              |
| 69:3G:103:LYS:N    | 69:3G:103:LYS:HD2  | 2.26                     | 0.51              |
| 71:3I:34:GLU:OE1   | 71:3I:34:GLU:C     | 2.54                     | 0.51              |
| 71:3I:35:TYR:CD1   | 71:3I:106:LEU:HB3  | 2.45                     | 0.51              |
| 75:3M:115:GLU:OE2  | 75:3M:119:LYS:HE3  | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:3N:7:ILE:HG23   | 76:3N:25:ILE:CG2   | 2.40                     | 0.51              |
| 77:3O:57:LYS:HA    | 77:3O:60:LYS:HG2   | 1.93                     | 0.51              |
| 79:3Q:52:LYS:NZ    | 79:3Q:52:LYS:HB3   | 2.24                     | 0.51              |
| 1:1A:34:A:OP1      | 16:2H:83:LYS:HB2   | 2.11                     | 0.51              |
| 1:1A:324:A:H2'     | 1:1A:325:U:H6      | 1.75                     | 0.51              |
| 1:1A:374:G:OP2     | 38:2d:56:ARG:NH1   | 2.39                     | 0.51              |
| 1:1A:424:U:H2'     | 1:1A:425:U:H6      | 1.75                     | 0.51              |
| 1:1A:518:G:H2'     | 1:1A:519:C:H5'     | 1.93                     | 0.51              |
| 1:1A:1701:A:H2'    | 1:1A:1701:A:N3     | 2.25                     | 0.51              |
| 1:1A:1768:C:H2'    | 1:1A:1771:U:O4     | 2.10                     | 0.51              |
| 1:1A:3900:G:OP1    | 1:1A:3901:A:O2'    | 2.11                     | 0.51              |
| 1:1A:3969:G:O2'    | 46:2l:207:LYS:HE3  | 2.10                     | 0.51              |
| 1:1A:4284:C:O2'    | 1:1A:4285:U:H5'    | 2.11                     | 0.51              |
| 1:1A:4460:U:H2'    | 1:1A:4461:C:C6     | 2.45                     | 0.51              |
| 3:1C:151:G:O2'     | 3:1C:152:U:H5'     | 2.11                     | 0.51              |
| 4:1D:30:ARG:HG3    | 4:1D:36:GLU:OE1    | 2.10                     | 0.51              |
| 4:1D:206:PRO:HD3   | 4:1D:213:GLY:CA    | 2.41                     | 0.51              |
| 6:1F:288:ASP:OD2   | 6:1F:291:ARG:HB2   | 2.11                     | 0.51              |
| 25:2Q:37:GLU:O     | 25:2Q:41:LEU:HG    | 2.11                     | 0.51              |
| 46:2l:59:PRO:CB    | 46:2l:170:GLY:HA3  | 2.38                     | 0.51              |
| 47:2m:86:C:H5'     | 47:2m:149:A:O2'    | 2.11                     | 0.51              |
| 47:2m:324:C:H1'    | 47:2m:327:G:H22    | 1.76                     | 0.51              |
| 47:2m:338:G:C2'    | 47:2m:339:A:H5'    | 2.40                     | 0.51              |
| 47:2m:540:U:H5'    | 47:2m:542:U:OP2    | 2.11                     | 0.51              |
| 47:2m:552:G:H2'    | 47:2m:553:U:C2     | 2.46                     | 0.51              |
| 47:2m:947:G:H2'    | 47:2m:948:C:H6     | 1.75                     | 0.51              |
| 47:2m:1512:C:HO2'  | 47:2m:1513:C:H6    | 1.58                     | 0.51              |
| 50:2p:53:THR:HG22  | 50:2p:91:VAL:CG2   | 2.41                     | 0.51              |
| 51:2q:11:ARG:NH1   | 51:2q:20:LEU:HB3   | 2.26                     | 0.51              |
| 53:2s:166:VAL:HG23 | 53:2s:166:VAL:O    | 2.10                     | 0.51              |
| 59:2y:69:ILE:O     | 59:2y:69:ILE:HG22  | 2.10                     | 0.51              |
| 62:21:31:SER:HB2   | 62:21:107:GLU:OE2  | 2.10                     | 0.51              |
| 68:3F:143:GLN:O    | 68:3F:144:ASP:HB3  | 2.09                     | 0.51              |
| 68:3F:236:ILE:HD12 | 68:3F:237:ASN:H    | 1.74                     | 0.51              |
| 72:3J:49:LEU:CD2   | 72:3J:123:VAL:HG11 | 2.39                     | 0.51              |
| 78:3P:67:THR:OG1   | 78:3P:68:GLY:N     | 2.44                     | 0.51              |
| 1:1A:423:G:H2'     | 1:1A:424:U:H6      | 1.75                     | 0.51              |
| 1:1A:1784:U:H4'    | 12:2D:90:ARG:O     | 2.10                     | 0.51              |
| 1:1A:1802:A:N3     | 22:2N:130:ARG:NH2  | 2.52                     | 0.51              |
| 1:1A:2504:C:H5'    | 26:2R:47:ARG:HH12  | 1.74                     | 0.51              |
| 1:1A:3702:A:O2'    | 1:1A:3774:A:OP1    | 2.16                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4317:A:O2'   | 1:1A:4318:C:O5'    | 2.23                     | 0.51              |
| 1:1A:4709:U:O2    | 1:1A:4709:U:H2'    | 2.11                     | 0.51              |
| 11:2C:173:ARG:HB3 | 41:2g:127:VAL:CG1  | 2.40                     | 0.51              |
| 13:2E:81:GLU:O    | 13:2E:85:LYS:HG3   | 2.10                     | 0.51              |
| 15:2G:86:TRP:O    | 15:2G:87:ALA:HB3   | 2.11                     | 0.51              |
| 21:2M:48:VAL:CG1  | 21:2M:54:MET:HB3   | 2.41                     | 0.51              |
| 25:2Q:44:ARG:HD3  | 25:2Q:49:ILE:HD11  | 1.93                     | 0.51              |
| 41:2g:92:ASP:O    | 41:2g:93:LYS:HG3   | 2.09                     | 0.51              |
| 43:2i:14:LYS:HG2  | 43:2i:15:CYS:N     | 2.25                     | 0.51              |
| 46:2l:179:LEU:CD2 | 46:2l:183:ILE:HD11 | 2.41                     | 0.51              |
| 47:2m:306:C:H4'   | 47:2m:309:G:OP1    | 2.11                     | 0.51              |
| 47:2m:325:C:H3'   | 47:2m:326:C:H5'    | 1.93                     | 0.51              |
| 47:2m:1049:A:OP2  | 47:2m:1068:G:N1    | 2.28                     | 0.51              |
| 47:2m:1203:G:O2'  | 47:2m:1204:A:H5'   | 2.11                     | 0.51              |
| 47:2m:1241:A:H5'' | 47:2m:1242:U:OP2   | 2.11                     | 0.51              |
| 47:2m:1283:C:H5'  | 47:2m:1284:A:O5'   | 2.11                     | 0.51              |
| 47:2m:1287:A:N1   | 47:2m:1312:G:H1'   | 2.26                     | 0.51              |
| 47:2m:1418:C:H1'  | 47:2m:1419:C:H2'   | 1.93                     | 0.51              |
| 47:2m:1518:C:O2   | 47:2m:1518:C:H3'   | 2.11                     | 0.51              |
| 47:2m:1537:A:C2'  | 47:2m:1538:C:H5'   | 2.41                     | 0.51              |
| 49:2o:185:VAL:HA  | 49:2o:188:LEU:CG   | 2.40                     | 0.51              |
| 51:2q:48:LEU:HD22 | 51:2q:52:LEU:HD12  | 1.93                     | 0.51              |
| 53:2s:11:PRO:HD3  | 53:2s:44:ASN:ND2   | 2.26                     | 0.51              |
| 57:2w:56:LEU:O    | 57:2w:60:LEU:CD2   | 2.58                     | 0.51              |
| 59:2y:16:ILE:CG2  | 59:2y:17:ILE:HD13  | 2.40                     | 0.51              |
| 60:2z:115:LYS:HG3 | 60:2z:116:LYS:N    | 2.26                     | 0.51              |
| 60:2z:121:ARG:HG3 | 60:2z:125:HIS:CD2  | 2.46                     | 0.51              |
| 61:20:11:GLN:OE1  | 61:20:11:GLN:HA    | 2.10                     | 0.51              |
| 61:20:72:VAL:O    | 61:20:76:THR:HG23  | 2.11                     | 0.51              |
| 65:3C:49:ALA:HB2  | 74:3L:117:ARG:NH2  | 2.25                     | 0.51              |
| 68:3F:172:LYS:HG2 | 68:3F:193:GLY:O    | 2.11                     | 0.51              |
| 69:3G:62:PRO:CD   | 69:3G:71:LYS:HD3   | 2.41                     | 0.51              |
| 69:3G:121:ARG:O   | 69:3G:121:ARG:HG3  | 2.10                     | 0.51              |
| 69:3G:153:GLY:O   | 69:3G:157:LEU:HD23 | 2.11                     | 0.51              |
| 71:3I:28:GLU:HG3  | 71:3I:40:LYS:HE2   | 1.93                     | 0.51              |
| 78:3P:75:GLU:HA   | 78:3P:75:GLU:OE1   | 2.10                     | 0.51              |
| 1:1A:189:G:H1'    | 1:1A:253:G:H22     | 1.76                     | 0.51              |
| 1:1A:417:G:C1'    | 1:1A:418:A:OP2     | 2.57                     | 0.51              |
| 1:1A:444:G:H1     | 1:1A:1303:A:H2     | 1.58                     | 0.51              |
| 1:1A:496:G:H2'    | 1:1A:498:C:OP1     | 2.10                     | 0.51              |
| 1:1A:1551:C:H2'   | 1:1A:1552:G:H5'    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1577:G:H5'   | 1:1A:1578:U:H5''   | 1.93                     | 0.51              |
| 1:1A:1690:C:H2'   | 1:1A:1691:G:O4'    | 2.11                     | 0.51              |
| 1:1A:1941:A:C2    | 1:1A:4434:C:H5'    | 2.46                     | 0.51              |
| 1:1A:1993:C:O2    | 1:1A:2002:A:N6     | 2.44                     | 0.51              |
| 1:1A:2267:U:P     | 45:2k:37:SER:HB2   | 2.51                     | 0.51              |
| 1:1A:2276:A:H2'   | 1:1A:2277:C:O4'    | 2.11                     | 0.51              |
| 1:1A:2337:C:H4'   | 45:2k:19:LYS:HB2   | 1.92                     | 0.51              |
| 1:1A:2759:G:O2'   | 1:1A:2760:G:H5'    | 2.11                     | 0.51              |
| 1:1A:4192:A:H2'   | 1:1A:4193:C:H6     | 1.76                     | 0.51              |
| 1:1A:4208:U:OP2   | 22:2N:4:THR:OG1    | 2.26                     | 0.51              |
| 1:1A:4233:A:C4'   | 43:2i:98:LYS:HE2   | 2.30                     | 0.51              |
| 1:1A:4348:A:O3'   | 1:1A:4349:C:H4'    | 2.11                     | 0.51              |
| 1:1A:4740:G:C6    | 1:1A:4741:C:H1'    | 2.45                     | 0.51              |
| 3:1C:43:A:O2'     | 3:1C:44:A:H5'      | 2.10                     | 0.51              |
| 18:2J:4:TYR:CZ    | 18:2J:16:LYS:HB2   | 2.46                     | 0.51              |
| 30:2V:25:ARG:HA   | 30:2V:25:ARG:HH11  | 1.75                     | 0.51              |
| 40:2f:34:LYS:HG3  | 40:2f:34:LYS:O     | 2.11                     | 0.51              |
| 47:2m:183:G:C4'   | 47:2m:184:G:H5'    | 2.41                     | 0.51              |
| 47:2m:398:A:C3'   | 47:2m:399:C:H5''   | 2.40                     | 0.51              |
| 47:2m:1447:G:H2'  | 47:2m:1448:A:C8    | 2.45                     | 0.51              |
| 47:2m:1451:G:OP1  | 59:2y:33:ARG:NH2   | 2.29                     | 0.51              |
| 47:2m:1518:C:OP1  | 47:2m:1519:U:H2'   | 2.11                     | 0.51              |
| 47:2m:1601:A:H5'' | 47:2m:1602:U:P     | 2.51                     | 0.51              |
| 47:2m:1621:U:H4'  | 57:2w:118:GLU:OE1  | 2.11                     | 0.51              |
| 52:2r:39:ILE:O    | 52:2r:39:ILE:HG22  | 2.11                     | 0.51              |
| 53:2s:126:HIS:ND1 | 53:2s:183:LYS:HE2  | 2.25                     | 0.51              |
| 54:2t:19:LYS:HB3  | 54:2t:19:LYS:HZ2   | 1.76                     | 0.51              |
| 54:2t:148:LYS:HA  | 54:2t:151:GLU:CG   | 2.41                     | 0.51              |
| 61:20:108:GLU:HG2 | 61:20:113:VAL:O    | 2.11                     | 0.51              |
| 66:3D:20:ARG:HA   | 66:3D:27:CYS:O     | 2.11                     | 0.51              |
| 71:3I:33:GLY:HA3  | 79:3Q:38:TYR:CG    | 2.46                     | 0.51              |
| 72:3J:17:ALA:HA   | 72:3J:20:GLU:HG2   | 1.92                     | 0.51              |
| 76:3N:35:VAL:HG22 | 76:3N:40:ILE:CG1   | 2.40                     | 0.51              |
| 77:3O:81:GLY:O    | 77:3O:85:ARG:HG3   | 2.11                     | 0.51              |
| 1:1A:387:G:OP1    | 1:1A:387:G:H4'     | 2.11                     | 0.51              |
| 1:1A:456:C:OP2    | 1:1A:456:C:H2'     | 2.11                     | 0.51              |
| 1:1A:498:C:H42    | 1:1A:656:C:H42     | 1.59                     | 0.51              |
| 1:1A:1803:G:C5    | 22:2N:109:VAL:HG22 | 2.46                     | 0.51              |
| 1:1A:1866:U:H2'   | 1:1A:1867:A:O4'    | 2.11                     | 0.51              |
| 1:1A:2362:U:H2'   | 1:1A:2362:U:O2     | 2.11                     | 0.51              |
| 1:1A:2729:C:O2'   | 1:1A:2730:U:H5'    | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2744:A:H2'    | 1:1A:2745:A:H8     | 1.74                     | 0.51              |
| 1:1A:2775:C:H2'    | 1:1A:2776:G:H8     | 1.76                     | 0.51              |
| 1:1A:3770:U:H2'    | 1:1A:3771:C:O4'    | 2.11                     | 0.51              |
| 1:1A:3970:G:H2'    | 1:1A:3971:G:C8     | 2.46                     | 0.51              |
| 1:1A:4438:U:H2'    | 1:1A:4439:U:O4'    | 2.11                     | 0.51              |
| 1:1A:4615:C:H5''   | 5:1E:357:ARG:NH1   | 2.26                     | 0.51              |
| 1:1A:4753:U:C5     | 8:1H:279:ASN:HB2   | 2.45                     | 0.51              |
| 1:1A:4760:G:H2'    | 1:1A:4761:G:H8     | 1.76                     | 0.51              |
| 2:1B:25:G:O2'      | 2:1B:26:C:H5'      | 2.10                     | 0.51              |
| 3:1C:18:U:H2'      | 3:1C:19:C:C6       | 2.46                     | 0.51              |
| 4:1D:129:ALA:HB3   | 4:1D:132:ASN:OD1   | 2.11                     | 0.51              |
| 5:1E:168:MET:CG    | 5:1E:178:ALA:HA    | 2.41                     | 0.51              |
| 6:1F:288:ASP:O     | 6:1F:292:ILE:HG13  | 2.11                     | 0.51              |
| 14:2F:47:ALA:HB3   | 14:2F:48:PRO:CD    | 2.31                     | 0.51              |
| 14:2F:154:VAL:HG12 | 14:2F:155:MET:HG3  | 1.93                     | 0.51              |
| 20:2L:84:THR:CG2   | 20:2L:87:ALA:H     | 2.24                     | 0.51              |
| 22:2N:115:LYS:CD   | 22:2N:126:VAL:HG11 | 2.37                     | 0.51              |
| 23:2O:76:VAL:HB    | 23:2O:77:PRO:CD    | 2.41                     | 0.51              |
| 23:2O:80:LYS:O     | 23:2O:110:TYR:HE2  | 1.94                     | 0.51              |
| 35:2a:40:LYS:HD3   | 35:2a:52:ARG:NH2   | 2.25                     | 0.51              |
| 47:2m:1173:A:O2'   | 47:2m:1174:U:H5'   | 2.11                     | 0.51              |
| 47:2m:1388:A:H61   | 50:2p:161:GLY:CA   | 2.23                     | 0.51              |
| 48:2n:107:THR:HA   | 48:2n:113:GLN:NE2  | 2.26                     | 0.51              |
| 51:2q:118:GLU:HG2  | 51:2q:121:TYR:HE1  | 1.75                     | 0.51              |
| 53:2s:6:ALA:O      | 53:2s:28:LEU:HD22  | 2.11                     | 0.51              |
| 53:2s:53:VAL:HG21  | 53:2s:172:THR:HA   | 1.92                     | 0.51              |
| 54:2t:46:VAL:HG13  | 54:2t:54:LYS:HG3   | 1.92                     | 0.51              |
| 55:2u:62:PHE:CZ    | 55:2u:65:ARG:HA    | 2.46                     | 0.51              |
| 59:2y:56:HIS:HA    | 59:2y:59:LYS:HE2   | 1.93                     | 0.51              |
| 62:21:43:ALA:HB1   | 62:21:50:VAL:HG22  | 1.91                     | 0.51              |
| 70:3H:68:LEU:HA    | 70:3H:100:CYS:SG   | 2.50                     | 0.51              |
| 1:1A:481:G:H2'     | 1:1A:482:G:H8      | 1.76                     | 0.50              |
| 1:1A:718:C:OP1     | 9:2A:217:ARG:NH1   | 2.44                     | 0.50              |
| 1:1A:1532:G:OP2    | 38:2d:31:LYS:NZ    | 2.40                     | 0.50              |
| 1:1A:1558:A:H2'    | 1:1A:1559:G:C8     | 2.46                     | 0.50              |
| 1:1A:1855:G:H2'    | 1:1A:1856:C:H6     | 1.76                     | 0.50              |
| 1:1A:1982:G:H4'    | 1:1A:2009:A:O2'    | 2.11                     | 0.50              |
| 1:1A:2050:G:O2'    | 1:1A:2051:C:H5'    | 2.10                     | 0.50              |
| 1:1A:2261:G:H4'    | 8:1H:112:MET:HE1   | 1.92                     | 0.50              |
| 1:1A:2404:A:H61    | 1:1A:2787:A:N6     | 2.09                     | 0.50              |
| 1:1A:2457:G:H21    | 1:1A:3672:G:N2     | 2.09                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2478:C:H2'    | 1:1A:2479:G:O4'    | 2.11                     | 0.50              |
| 1:1A:2525:U:H2'    | 1:1A:2527:A:OP2    | 2.11                     | 0.50              |
| 1:1A:2871:A:H2'    | 1:1A:2872:C:O4'    | 2.11                     | 0.50              |
| 1:1A:3653:A:P      | 1:1A:3653:A:H8     | 2.34                     | 0.50              |
| 1:1A:3810:C:H4'    | 1:1A:3811:G:OP2    | 2.09                     | 0.50              |
| 6:1F:60:HIS:NE2    | 6:1F:100:ARG:HD3   | 2.26                     | 0.50              |
| 8:1H:50:LEU:H      | 8:1H:50:LEU:CD2    | 2.24                     | 0.50              |
| 15:2G:96:GLU:O     | 15:2G:100:ARG:HG2  | 2.11                     | 0.50              |
| 35:2a:46:CYS:SG    | 35:2a:48:VAL:HG22  | 2.51                     | 0.50              |
| 46:2l:66:CYS:O     | 46:2l:111:LEU:HD22 | 2.11                     | 0.50              |
| 47:2m:84:A:H2'     | 47:2m:85:A:O4'     | 2.10                     | 0.50              |
| 47:2m:693:A:H2'    | 47:2m:694:G:C5'    | 2.32                     | 0.50              |
| 47:2m:807:G:O2'    | 47:2m:808:A:H5'    | 2.10                     | 0.50              |
| 47:2m:811:A:HO2'   | 47:2m:812:A:P      | 2.32                     | 0.50              |
| 47:2m:812:A:C2     | 47:2m:813:A:H1'    | 2.46                     | 0.50              |
| 47:2m:1074:C:O2'   | 47:2m:1075:C:H5'   | 2.11                     | 0.50              |
| 47:2m:1144:A:H5'   | 47:2m:1355:C:N4    | 2.16                     | 0.50              |
| 47:2m:1471:C:H2'   | 47:2m:1472:C:O4'   | 2.11                     | 0.50              |
| 47:2m:1665:G:C2    | 61:20:87:VAL:HG12  | 2.46                     | 0.50              |
| 49:2o:32:ASP:OD2   | 49:2o:34:LYS:HE2   | 2.11                     | 0.50              |
| 51:2q:122:LYS:CG   | 51:2q:162:ILE:HD11 | 2.39                     | 0.50              |
| 51:2q:200:ARG:HA   | 51:2q:206:ASP:CG   | 2.35                     | 0.50              |
| 52:2r:87:LEU:HB3   | 58:2x:46:THR:HG21  | 1.93                     | 0.50              |
| 53:2s:158:LEU:HB2  | 53:2s:189:PHE:CD2  | 2.45                     | 0.50              |
| 53:2s:158:LEU:HD12 | 53:2s:189:PHE:CE2  | 2.46                     | 0.50              |
| 57:2w:51:ARG:O     | 57:2w:55:SER:OG    | 2.28                     | 0.50              |
| 59:2y:97:GLU:OE1   | 59:2y:97:GLU:HA    | 2.10                     | 0.50              |
| 61:20:60:THR:HG22  | 61:20:107:LEU:HD11 | 1.92                     | 0.50              |
| 64:3B:70:VAL:HG11  | 64:3B:94:ILE:HG21  | 1.93                     | 0.50              |
| 65:3C:78:ALA:HB1   | 65:3C:84:VAL:HG22  | 1.93                     | 0.50              |
| 69:3G:168:GLY:N    | 69:3G:179:THR:O    | 2.39                     | 0.50              |
| 75:3M:83:LEU:HD21  | 75:3M:121:THR:C    | 2.35                     | 0.50              |
| 1:1A:120:A:H4'     | 1:1A:121:A:H5'     | 1.93                     | 0.50              |
| 1:1A:261:G:H2'     | 1:1A:262:G:H8      | 1.76                     | 0.50              |
| 1:1A:444:G:O2'     | 1:1A:445:U:H5'     | 2.10                     | 0.50              |
| 1:1A:1431:C:C2'    | 1:1A:1432:G:H5'    | 2.40                     | 0.50              |
| 1:1A:1459:A:OP1    | 19:2K:65:ARG:NH1   | 2.45                     | 0.50              |
| 1:1A:1495:G:C2'    | 1:1A:1496:G:H5'    | 2.41                     | 0.50              |
| 1:1A:1560:A:O2'    | 1:1A:1561:G:H5'    | 2.11                     | 0.50              |
| 1:1A:1577:G:C2     | 1:1A:3637:U:H1'    | 2.46                     | 0.50              |
| 1:1A:1978:C:H4'    | 1:1A:1990:A:N1     | 2.26                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2027:U:O2'   | 1:1A:2028:C:H5'    | 2.11                     | 0.50              |
| 1:1A:2400:G:H21   | 35:2a:6:THR:HG22   | 1.76                     | 0.50              |
| 1:1A:2607:C:H2'   | 1:1A:2608:G:H8     | 1.76                     | 0.50              |
| 1:1A:2608:G:H2'   | 1:1A:2609:G:H8     | 1.75                     | 0.50              |
| 1:1A:4290:U:OP1   | 43:2i:9[B]:ARG:NH1 | 2.45                     | 0.50              |
| 4:1D:20:VAL:HA    | 4:1D:23:ARG:HG3    | 1.91                     | 0.50              |
| 4:1D:179:ILE:HG23 | 4:1D:184:ARG:HB2   | 1.93                     | 0.50              |
| 4:1D:248:GLY:O    | 4:1D:249:THR:OG1   | 2.21                     | 0.50              |
| 8:1H:223:ARG:CZ   | 8:1H:234:ASP:HB2   | 2.40                     | 0.50              |
| 8:1H:235:THR:HG23 | 8:1H:236:GLU:OE2   | 2.11                     | 0.50              |
| 9:2A:143:GLY:HA3  | 9:2A:240:ILE:HB    | 1.93                     | 0.50              |
| 13:2E:64:ARG:O    | 13:2E:65:ASN:HB2   | 2.11                     | 0.50              |
| 23:2O:48:LYS:HA   | 23:2O:52:LYS:O     | 2.11                     | 0.50              |
| 25:2Q:114:GLU:O   | 25:2Q:117:LYS:HD3  | 2.10                     | 0.50              |
| 26:2R:54:LEU:HD23 | 26:2R:54:LEU:H     | 1.77                     | 0.50              |
| 28:2T:4:PHE:O     | 28:2T:9:LYS:HG3    | 2.10                     | 0.50              |
| 47:2m:79:A:H2'    | 47:2m:80:G:C5'     | 2.41                     | 0.50              |
| 47:2m:177:G:N2    | 47:2m:313:A:O2'    | 2.44                     | 0.50              |
| 47:2m:302:A:H1'   | 54:2t:73:THR:HG23  | 1.92                     | 0.50              |
| 47:2m:336:A:H2'   | 47:2m:337:C:H6     | 1.77                     | 0.50              |
| 47:2m:341:C:O2'   | 47:2m:342:C:H5'    | 2.11                     | 0.50              |
| 47:2m:481:C:H2'   | 47:2m:482:G:H1'    | 1.93                     | 0.50              |
| 47:2m:527:C:H2'   | 47:2m:528:A:H8     | 1.76                     | 0.50              |
| 47:2m:896:U:H5'   | 47:2m:897:U:OP2    | 2.11                     | 0.50              |
| 47:2m:1143:A:O3'  | 47:2m:1355:C:N4    | 2.44                     | 0.50              |
| 47:2m:1192:U:P    | 64:3B:119:ARG:HH22 | 2.34                     | 0.50              |
| 47:2m:1281:G:C2'  | 47:2m:1282:A:OP2   | 2.58                     | 0.50              |
| 47:2m:1550:G:O2'  | 47:2m:1558:C:O2    | 2.05                     | 0.50              |
| 47:2m:1606:G:N2   | 47:2m:1632:G:H2'   | 2.26                     | 0.50              |
| 48:2n:42:LYS:HB3  | 48:2n:44:ASP:OD1   | 2.12                     | 0.50              |
| 51:2q:159:THR:HB  | 51:2q:173:ILE:HG12 | 1.90                     | 0.50              |
| 51:2q:181:CYS:CB  | 51:2q:195:ILE:HD11 | 2.40                     | 0.50              |
| 58:2x:50:LYS:CA   | 58:2x:53:GLU:HG3   | 2.42                     | 0.50              |
| 59:2y:115:SER:HB2 | 59:2y:117:LEU:CD1  | 2.42                     | 0.50              |
| 66:3D:15:THR:HG23 | 66:3D:16:LYS:N     | 2.26                     | 0.50              |
| 66:3D:18:LEU:CB   | 66:3D:29:GLN:HB2   | 2.41                     | 0.50              |
| 68:3F:280:LYS:O   | 68:3F:280:LYS:HG2  | 2.10                     | 0.50              |
| 69:3G:272:HIS:O   | 69:3G:276:THR:OG1  | 2.26                     | 0.50              |
| 70:3H:137:ARG:HD3 | 70:3H:140:ARG:NE   | 2.26                     | 0.50              |
| 71:3I:120:ALA:HB1 | 71:3I:125:HIS:ND1  | 2.26                     | 0.50              |
| 72:3J:44:LYS:HA   | 72:3J:44:LYS:HE2   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 75:3M:40:VAL:HA    | 75:3M:43:LYS:HE2  | 1.92                     | 0.50              |
| 76:3N:11:LYS:HB2   | 76:3N:24:VAL:HG23 | 1.93                     | 0.50              |
| 1:1A:139:G:H2'     | 1:1A:140:G:C1'    | 2.41                     | 0.50              |
| 1:1A:264:C:H2'     | 1:1A:265:C:C2     | 2.46                     | 0.50              |
| 1:1A:448:G:H3'     | 1:1A:449:C:C5'    | 2.41                     | 0.50              |
| 1:1A:660:A:H2'     | 1:1A:661:C:C6     | 2.46                     | 0.50              |
| 1:1A:1167:C:H2'    | 1:1A:1168:G:O4'   | 2.11                     | 0.50              |
| 1:1A:1381:U:H2'    | 1:1A:1382:G:H5'   | 1.93                     | 0.50              |
| 1:1A:2695:A:C5'    | 39:2e:26:LYS:HE3  | 2.38                     | 0.50              |
| 1:1A:2705:G:H2'    | 1:1A:2705:G:N3    | 2.26                     | 0.50              |
| 1:1A:3707:U:H2'    | 1:1A:3708:C:C6    | 2.46                     | 0.50              |
| 1:1A:3793:U:H2'    | 1:1A:3794:C:C6    | 2.47                     | 0.50              |
| 1:1A:3890:A:H2'    | 1:1A:3891:A:H5'   | 1.93                     | 0.50              |
| 1:1A:3928:A:H2'    | 1:1A:3929:G:O4'   | 2.12                     | 0.50              |
| 1:1A:4643:G:O2'    | 1:1A:4644:G:H5'   | 2.12                     | 0.50              |
| 1:1A:4710:C:H2'    | 1:1A:4711:C:C6    | 2.45                     | 0.50              |
| 1:1A:4732:G:H5''   | 1:1A:4733:C:H5''  | 1.93                     | 0.50              |
| 40:2f:44:TRP:CH2   | 40:2f:45:ARG:HD2  | 2.46                     | 0.50              |
| 46:2l:54:ARG:HA    | 46:2l:154:THR:CB  | 2.42                     | 0.50              |
| 46:2l:191:VAL:HG11 | 46:2l:200:ASN:OD1 | 2.11                     | 0.50              |
| 47:2m:502:C:H3'    | 47:2m:503:C:C6    | 2.46                     | 0.50              |
| 47:2m:600:G:H2'    | 47:2m:601:G:H8    | 1.76                     | 0.50              |
| 47:2m:1422:G:H2'   | 47:2m:1424:G:OP2  | 2.10                     | 0.50              |
| 47:2m:1544:C:H2'   | 47:2m:1545:A:H5'' | 1.94                     | 0.50              |
| 47:2m:1563:G:H2'   | 47:2m:1564:C:C6   | 2.47                     | 0.50              |
| 47:2m:1647:A:N1    | 47:2m:1675:A:H5'' | 2.26                     | 0.50              |
| 47:2m:1794:C:H2'   | 47:2m:1795:G:C8   | 2.46                     | 0.50              |
| 49:2o:82:ARG:CD    | 49:2o:103:MET:HE3 | 2.40                     | 0.50              |
| 50:2p:190:LEU:HD12 | 50:2p:200:PRO:CD  | 2.41                     | 0.50              |
| 52:2r:20:PHE:CZ    | 52:2r:94:LYS:HD3  | 2.41                     | 0.50              |
| 52:2r:162:ALA:HB2  | 52:2r:169:ILE:HA  | 1.92                     | 0.50              |
| 52:2r:193:LYS:HD2  | 52:2r:197:GLU:CG  | 2.41                     | 0.50              |
| 53:2s:75:ILE:CD1   | 53:2s:79:LEU:HD11 | 2.41                     | 0.50              |
| 53:2s:145:ARG:O    | 53:2s:152:ARG:HA  | 2.11                     | 0.50              |
| 53:2s:148:LEU:HD22 | 75:3M:42:MET:HG2  | 1.92                     | 0.50              |
| 60:2z:6:PRO:HD2    | 77:3O:49:LEU:HD13 | 1.92                     | 0.50              |
| 70:3H:109:LEU:HD23 | 70:3H:109:LEU:C   | 2.37                     | 0.50              |
| 80:3R:103:LEU:HB3  | 80:3R:105:TYR:CE1 | 2.46                     | 0.50              |
| 1:1A:37:U:H2'      | 1:1A:38:A:O4'     | 2.10                     | 0.50              |
| 1:1A:294:G:OP2     | 1:1A:296:A:O2'    | 2.25                     | 0.50              |
| 1:1A:1470:G:O2'    | 1:1A:1471:U:H5'   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2588:C:OP2   | 1:1A:2769:U:H5''   | 2.11                     | 0.50              |
| 1:1A:4753:U:H5    | 8:1H:279:ASN:H     | 1.58                     | 0.50              |
| 1:1A:5016:A:H5''  | 1:1A:5017:G:OP2    | 2.11                     | 0.50              |
| 6:1F:186:SER:O    | 6:1F:188:ARG:HD3   | 2.12                     | 0.50              |
| 7:1G:150:LEU:CD1  | 13:2E:146:ARG:HG3  | 2.41                     | 0.50              |
| 13:2E:36:ALA:HA   | 13:2E:39:VAL:HG12  | 1.92                     | 0.50              |
| 21:2M:102:THR:O   | 21:2M:106:VAL:HG23 | 2.11                     | 0.50              |
| 27:2S:54:GLU:HG3  | 27:2S:108:ARG:HB3  | 1.92                     | 0.50              |
| 33:2Y:77:PHE:CE1  | 45:2k:20:ARG:HG3   | 2.46                     | 0.50              |
| 45:2k:46:ARG:O    | 45:2k:65:LYS:HD3   | 2.11                     | 0.50              |
| 47:2m:106:C:OP1   | 47:2m:432:G:H5'    | 2.11                     | 0.50              |
| 47:2m:594:A:H4'   | 47:2m:595:U:H5'    | 1.93                     | 0.50              |
| 47:2m:792:C:N3    | 47:2m:793:G:N2     | 2.59                     | 0.50              |
| 47:2m:1119:A:H3'  | 47:2m:1119:A:N3    | 2.27                     | 0.50              |
| 47:2m:1284:A:H61  | 72:3J:33:ARG:HD3   | 1.77                     | 0.50              |
| 47:2m:1301:A:H4'  | 67:3E:3:HIS:CE1    | 2.47                     | 0.50              |
| 47:2m:1361:G:OP1  | 47:2m:1363:C:H5'   | 2.11                     | 0.50              |
| 47:2m:1439:A:H2'  | 47:2m:1440:C:C6    | 2.47                     | 0.50              |
| 47:2m:1505:U:H1'  | 47:2m:1508:A:N3    | 2.26                     | 0.50              |
| 47:2m:1563:G:H2'  | 47:2m:1564:C:H6    | 1.77                     | 0.50              |
| 47:2m:1771:G:H3'  | 47:2m:1771:G:N3    | 2.26                     | 0.50              |
| 47:2m:1865:C:C2   | 65:3C:5:ARG:HB3    | 2.46                     | 0.50              |
| 52:2r:42:LYS:HE3  | 52:2r:42:LYS:HA    | 1.94                     | 0.50              |
| 53:2s:15:LYS:N    | 53:2s:16:PRO:CD    | 2.66                     | 0.50              |
| 58:2x:89:SER:HB3  | 58:2x:112:LEU:CD1  | 2.41                     | 0.50              |
| 68:3F:37:ASP:O    | 68:3F:38:LYS:HD2   | 2.12                     | 0.50              |
| 68:3F:113:PHE:CD1 | 68:3F:120:ILE:HD13 | 2.47                     | 0.50              |
| 71:3I:122:SER:HB3 | 71:3I:125:HIS:CB   | 2.42                     | 0.50              |
| 76:3N:20:ARG:HD3  | 76:3N:76:TYR:HE1   | 1.76                     | 0.50              |
| 76:3N:55:ILE:N    | 76:3N:55:ILE:HD12  | 2.27                     | 0.50              |
| 1:1A:31:U:O2'     | 1:1A:32:G:H5'      | 2.11                     | 0.50              |
| 1:1A:4423:U:H3'   | 41:2g:97:ARG:NH2   | 2.24                     | 0.50              |
| 1:1A:4481:U:H2'   | 1:1A:4482:U:H6     | 1.76                     | 0.50              |
| 1:1A:4529:G:OP1   | 81:1A:5110:84D:N3  | 2.44                     | 0.50              |
| 1:1A:4944:C:OP1   | 34:2Z:104:MET:HE3  | 2.12                     | 0.50              |
| 1:1A:5063:G:O6    | 5:1E:124:LYS:NZ    | 2.35                     | 0.50              |
| 2:1B:40:U:O2      | 13:2E:75:ARG:NE    | 2.28                     | 0.50              |
| 3:1C:126:C:H1'    | 3:1C:127:U:O4'     | 2.11                     | 0.50              |
| 4:1D:101:VAL:HG22 | 4:1D:165:VAL:HG22  | 1.92                     | 0.50              |
| 5:1E:220:ILE:HG12 | 5:1E:278:THR:HG23  | 1.92                     | 0.50              |
| 25:2Q:14:TYR:HB3  | 25:2Q:15:PRO:CD    | 2.38                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:2R:116:LEU:C   | 26:2R:116:LEU:HD12 | 2.36                     | 0.50              |
| 31:2W:87:LYS:HB3  | 31:2W:89:TYR:CE1   | 2.46                     | 0.50              |
| 32:2X:50:ARG:HG2  | 32:2X:62:VAL:HG22  | 1.94                     | 0.50              |
| 46:2L:143:ASN:HA  | 46:2L:148:VAL:CG1  | 2.41                     | 0.50              |
| 47:2m:677:G:N1    | 47:2m:1027:A:OP2   | 2.40                     | 0.50              |
| 47:2m:753:C:H5''  | 47:2m:791:C:O2'    | 2.12                     | 0.50              |
| 47:2m:805:U:O2'   | 47:2m:806:U:H5'    | 2.12                     | 0.50              |
| 47:2m:888:U:H2'   | 47:2m:898:U:H3     | 1.77                     | 0.50              |
| 47:2m:894:G:H3'   | 47:2m:895:G:C5'    | 2.42                     | 0.50              |
| 47:2m:1412:C:H5'  | 47:2m:1413:G:P     | 2.51                     | 0.50              |
| 47:2m:1673:U:O2'  | 52:2r:84:GLY:O     | 2.18                     | 0.50              |
| 47:2m:1728:U:H2'  | 47:2m:1729:U:O4'   | 2.12                     | 0.50              |
| 48:2n:78:SER:HB2  | 48:2n:125:THR:OG1  | 2.11                     | 0.50              |
| 53:2s:31:GLU:CA   | 53:2s:37:LYS:HE3   | 2.42                     | 0.50              |
| 55:2u:19:GLY:O    | 55:2u:71:LEU:N     | 2.44                     | 0.50              |
| 59:2y:115:SER:HB2 | 59:2y:117:LEU:HG   | 1.93                     | 0.50              |
| 60:2z:118:ARG:CG  | 60:2z:118:ARG:O    | 2.59                     | 0.50              |
| 66:3D:14:VAL:HA   | 66:3D:32:VAL:HG12  | 1.92                     | 0.50              |
| 66:3D:14:VAL:HG11 | 66:3D:52:GLU:HA    | 1.94                     | 0.50              |
| 68:3F:142:VAL:CG1 | 68:3F:146:SER:HB2  | 2.41                     | 0.50              |
| 71:3I:141:VAL:CG1 | 76:3N:65:GLY:HA3   | 2.41                     | 0.50              |
| 77:3O:54:THR:HG22 | 77:3O:78:LYS:HD3   | 1.93                     | 0.50              |
| 1:1A:659:G:H2'    | 1:1A:660:A:C8      | 2.47                     | 0.50              |
| 1:1A:751:G:H2'    | 1:1A:752:G:O4'     | 2.12                     | 0.50              |
| 1:1A:1238:A:O2'   | 9:2A:52:GLU:OE2    | 2.30                     | 0.50              |
| 1:1A:1516:G:O2'   | 14:2F:18:TRP:NE1   | 2.38                     | 0.50              |
| 1:1A:2621:A:H2'   | 1:1A:2622:G:C8     | 2.47                     | 0.50              |
| 1:1A:3702:A:H2'   | 1:1A:3702:A:N3     | 2.26                     | 0.50              |
| 1:1A:3974:G:N1    | 1:1A:4050:A:H2'    | 2.18                     | 0.50              |
| 1:1A:4148:C:O2'   | 1:1A:4149:C:H5'    | 2.11                     | 0.50              |
| 1:1A:4260:U:H2'   | 1:1A:4261:C:H6     | 1.76                     | 0.50              |
| 1:1A:4481:U:H2'   | 1:1A:4482:U:C6     | 2.46                     | 0.50              |
| 1:1A:4935:C:H2'   | 1:1A:4936:G:C8     | 2.46                     | 0.50              |
| 3:1C:38:U:H3'     | 3:1C:39:G:H5'      | 1.92                     | 0.50              |
| 3:1C:137:A:H2'    | 3:1C:138:C:C6      | 2.46                     | 0.50              |
| 4:1D:14:SER:CA    | 4:1D:17:ARG:HE     | 2.21                     | 0.50              |
| 13:2E:20:LEU:CD2  | 13:2E:82:ILE:HB    | 2.42                     | 0.50              |
| 13:2E:31:ASP:O    | 13:2E:34:THR:HG22  | 2.11                     | 0.50              |
| 16:2H:158:HIS:HB3 | 16:2H:161:MET:HB2  | 1.93                     | 0.50              |
| 47:2m:508:A:H3'   | 47:2m:509:G:H8     | 1.77                     | 0.50              |
| 47:2m:986:G:C8    | 74:3L:137:SER:HA   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:1011:A:O2'  | 47:2m:1012:A:OP1   | 2.21                     | 0.50              |
| 47:2m:1201:U:H2'  | 47:2m:1202:U:C6    | 2.47                     | 0.50              |
| 47:2m:1398:G:O5'  | 68:3F:61:GLY:HA2   | 2.12                     | 0.50              |
| 47:2m:1442:U:H2'  | 47:2m:1443:C:H6    | 1.75                     | 0.50              |
| 47:2m:1596:U:P    | 77:3O:85:ARG:HH12  | 2.34                     | 0.50              |
| 47:2m:1807:C:H2'  | 47:2m:1808:U:O4'   | 2.12                     | 0.50              |
| 48:2n:107:THR:HA  | 48:2n:113:GLN:HE22 | 1.77                     | 0.50              |
| 49:2o:71:LEU:HG   | 49:2o:78:GLU:HB3   | 1.93                     | 0.50              |
| 50:2p:93:THR:HB   | 50:2p:96:LEU:HB2   | 1.94                     | 0.50              |
| 54:2t:113:TYR:OH  | 54:2t:156:ALA:O    | 2.30                     | 0.50              |
| 58:2x:143:LYS:HE3 | 58:2x:145:TYR:CE1  | 2.46                     | 0.50              |
| 59:2y:134:PRO:O   | 59:2y:135:VAL:HB   | 2.10                     | 0.50              |
| 60:2z:105:ASN:OD1 | 60:2z:108:ARG:HD3  | 2.12                     | 0.50              |
| 68:3F:135:LEU:H   | 68:3F:135:LEU:HD23 | 1.75                     | 0.50              |
| 69:3G:271:ASP:OD1 | 69:3G:272:HIS:N    | 2.43                     | 0.50              |
| 71:3I:127:ARG:HD3 | 79:3Q:31:ARG:HD3   | 1.92                     | 0.50              |
| 77:3O:98:LYS:CD   | 77:3O:110:THR:HG23 | 2.41                     | 0.50              |
| 1:1A:205:C:N3     | 1:1A:209:U:H5      | 2.09                     | 0.50              |
| 1:1A:970:G:H3'    | 1:1A:970:G:N3      | 2.26                     | 0.50              |
| 1:1A:1081:C:HO2'  | 1:1A:1219:G:H22    | 1.56                     | 0.50              |
| 1:1A:1730:U:H2'   | 1:1A:1731:C:C6     | 2.46                     | 0.50              |
| 1:1A:2540:C:H5''  | 35:2a:65:MET:CE    | 2.42                     | 0.50              |
| 1:1A:2629:C:H2'   | 1:1A:2630:U:O4'    | 2.12                     | 0.50              |
| 1:1A:2705:G:H1'   | 1:1A:2712:G:H22    | 1.75                     | 0.50              |
| 1:1A:4890:G:O2'   | 1:1A:4891:G:H5'    | 2.11                     | 0.50              |
| 3:1C:69:U:O2'     | 3:1C:70:G:H5'      | 2.12                     | 0.50              |
| 3:1C:70:G:H1'     | 3:1C:88:A:N6       | 2.27                     | 0.50              |
| 7:1G:93:THR:O     | 7:1G:158:LYS:HE3   | 2.12                     | 0.50              |
| 10:2B:153:GLN:O   | 10:2B:180:PRO:HG2  | 2.11                     | 0.50              |
| 11:2C:12:ILE:HD12 | 11:2C:53:LYS:HB3   | 1.92                     | 0.50              |
| 13:2E:175:LEU:HB3 | 13:2E:176:PRO:CD   | 2.41                     | 0.50              |
| 15:2G:126:GLU:HG3 | 17:2I:185:VAL:CG1  | 2.38                     | 0.50              |
| 29:2U:79:TRP:CZ3  | 29:2U:87:ARG:HG3   | 2.47                     | 0.50              |
| 38:2d:64:MET:O    | 38:2d:68:LYS:HG2   | 2.11                     | 0.50              |
| 43:2i:99:ARG:HD3  | 43:2i:100:LYS:N    | 2.26                     | 0.50              |
| 46:2l:58:THR:N    | 46:2l:59:PRO:HD3   | 2.27                     | 0.50              |
| 47:2m:1157:G:O2'  | 75:3M:76:SER:N     | 2.40                     | 0.50              |
| 47:2m:1227:G:H21  | 47:2m:1635:C:H4'   | 1.76                     | 0.50              |
| 47:2m:1628:C:H2'  | 47:2m:1629:C:H6    | 1.75                     | 0.50              |
| 47:2m:1792:G:H2'  | 47:2m:1793:A:H8    | 1.75                     | 0.50              |
| 47:2m:1866:A:N6   | 65:3C:84:VAL:HB    | 2.27                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:2n:26:GLY:O     | 48:2n:46:ILE:HG23  | 2.11                     | 0.50              |
| 52:2r:18:LYS:HG3   | 52:2r:21:GLY:HA2   | 1.94                     | 0.50              |
| 52:2r:142:SER:HB3  | 66:3D:46:VAL:HG21  | 1.93                     | 0.50              |
| 52:2r:165:ASN:ND2  | 52:2r:167:LYS:HD2  | 2.26                     | 0.50              |
| 54:2t:11:ARG:HD3   | 54:2t:15:GLY:O     | 2.12                     | 0.50              |
| 55:2u:31:LYS:HG2   | 55:2u:39:ASN:OD1   | 2.12                     | 0.50              |
| 59:2y:98:VAL:O     | 59:2y:119:VAL:HA   | 2.11                     | 0.50              |
| 60:2z:70:ILE:HG22  | 60:2z:77:TYR:CE2   | 2.46                     | 0.50              |
| 62:21:40:ILE:HG23  | 62:21:50:VAL:HG11  | 1.94                     | 0.50              |
| 63:3A:42:VAL:HG23  | 63:3A:43:THR:CG2   | 2.36                     | 0.50              |
| 68:3F:142:VAL:HG13 | 68:3F:146:SER:HB2  | 1.94                     | 0.50              |
| 68:3F:197:THR:HG21 | 68:3F:239:LEU:N    | 2.26                     | 0.50              |
| 69:3G:134:ASN:C    | 69:3G:167:ARG:HH12 | 2.19                     | 0.50              |
| 76:3N:94:HIS:NE2   | 76:3N:96:LEU:HD12  | 2.26                     | 0.50              |
| 77:3O:61:GLU:O     | 77:3O:64:ASN:HB2   | 2.11                     | 0.50              |
| 1:1A:128:C:C2'     | 1:1A:129:C:O4'     | 2.60                     | 0.50              |
| 1:1A:202:C:O2'     | 1:1A:203:U:H5'     | 2.11                     | 0.50              |
| 1:1A:374:G:H2'     | 1:1A:375:G:H5'     | 1.94                     | 0.50              |
| 1:1A:484:U:H4'     | 1:1A:485:C:H5''    | 1.91                     | 0.50              |
| 1:1A:736:C:O2'     | 1:1A:737:C:H5'     | 2.11                     | 0.50              |
| 1:1A:956:A:N6      | 1:1A:1283:G:H1'    | 2.26                     | 0.50              |
| 1:1A:1084:C:H2'    | 1:1A:1085:C:H6     | 1.75                     | 0.50              |
| 1:1A:1495:G:H2'    | 1:1A:1496:G:H5'    | 1.93                     | 0.50              |
| 1:1A:2260:C:H5''   | 1:1A:2261:G:H5'    | 1.92                     | 0.50              |
| 1:1A:2407:G:O6     | 40:2f:2:SER:N      | 2.44                     | 0.50              |
| 1:1A:3934:G:H2'    | 1:1A:3935:C:C6     | 2.47                     | 0.50              |
| 1:1A:3947:A:H2'    | 1:1A:3948:C:C5'    | 2.30                     | 0.50              |
| 1:1A:4511:A:H2'    | 1:1A:4512:U:O4'    | 2.12                     | 0.50              |
| 1:1A:4685:U:H2'    | 1:1A:4686:G:C8     | 2.46                     | 0.50              |
| 1:1A:5057:C:H2'    | 1:1A:5058:A:O4'    | 2.12                     | 0.50              |
| 11:2C:100:PRO:O    | 11:2C:116:ASN:HB3  | 2.11                     | 0.50              |
| 13:2E:32:ARG:HA    | 13:2E:126:TYR:OH   | 2.12                     | 0.50              |
| 17:2I:201:LEU:H    | 17:2I:201:LEU:HD12 | 1.77                     | 0.50              |
| 22:2N:41:ASP:OD1   | 22:2N:61:THR:OG1   | 2.17                     | 0.50              |
| 22:2N:115:LYS:CD   | 22:2N:126:VAL:HG21 | 2.37                     | 0.50              |
| 31:2W:81:LEU:HG    | 31:2W:91:VAL:CG2   | 2.41                     | 0.50              |
| 46:2l:110:PHE:HB2  | 46:2l:135:PRO:HG3  | 1.94                     | 0.50              |
| 47:2m:144:U:OP1    | 70:3H:139:SER:HB2  | 2.12                     | 0.50              |
| 47:2m:539:C:H5'    | 47:2m:540:U:C4'    | 2.41                     | 0.50              |
| 47:2m:885:U:H1'    | 47:2m:901:G:N2     | 2.26                     | 0.50              |
| 47:2m:949:G:H2'    | 47:2m:950:C:C6     | 2.46                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:2m:1461:G:N2    | 47:2m:1464:C:H3'  | 2.27                     | 0.50              |
| 47:2m:1481:G:H2'   | 47:2m:1482:C:C6   | 2.47                     | 0.50              |
| 47:2m:1736:G:H2'   | 47:2m:1737:G:H8   | 1.77                     | 0.50              |
| 48:2n:176:TRP:HA   | 48:2n:202:TYR:CE2 | 2.47                     | 0.50              |
| 49:2o:44:ILE:HD12  | 49:2o:45:GLY:N    | 2.26                     | 0.50              |
| 49:2o:49:VAL:CG1   | 49:2o:62:LEU:HD23 | 2.36                     | 0.50              |
| 50:2p:123:LEU:O    | 50:2p:127:MET:SD  | 2.70                     | 0.50              |
| 50:2p:146:ARG:NH1  | 50:2p:146:ARG:HB3 | 2.27                     | 0.50              |
| 55:2u:24:LYS:HG3   | 55:2u:26:ASP:CG   | 2.37                     | 0.50              |
| 55:2u:35:LEU:CD2   | 55:2u:40:VAL:HG23 | 2.42                     | 0.50              |
| 58:2x:93:VAL:HG11  | 58:2x:109:LYS:HZ2 | 1.76                     | 0.50              |
| 59:2y:60:ARG:HH22  | 59:2y:67:ARG:HG3  | 1.77                     | 0.50              |
| 61:20:27:LYS:HA    | 61:20:27:LYS:CE   | 2.41                     | 0.50              |
| 67:3E:3:HIS:H      | 67:3E:3:HIS:CD2   | 2.29                     | 0.50              |
| 68:3F:164:ILE:HD12 | 68:3F:164:ILE:O   | 2.11                     | 0.50              |
| 71:3I:35:TYR:CE1   | 71:3I:106:LEU:HB3 | 2.47                     | 0.50              |
| 73:3K:18:TYR:O     | 75:3M:56:HIS:ND1  | 2.45                     | 0.50              |
| 73:3K:38:TYR:HE1   | 73:3K:74:ILE:HG22 | 1.77                     | 0.50              |
| 73:3K:71:ILE:O     | 73:3K:75:LEU:HD23 | 2.11                     | 0.50              |
| 76:3N:97:TYR:OH    | 76:3N:99:LYS:HD3  | 2.12                     | 0.50              |
| 80:3R:140:TYR:HD1  | 80:3R:147:THR:HB  | 1.76                     | 0.50              |
| 1:1A:10:A:H2'      | 1:1A:11:G:H8      | 1.77                     | 0.50              |
| 1:1A:689:U:OP1     | 8:1H:107:VAL:HG13 | 2.12                     | 0.50              |
| 1:1A:1071:C:H5''   | 1:1A:1072:C:OP1   | 2.11                     | 0.50              |
| 1:1A:1273:G:C6     | 8:1H:73:TYR:HB2   | 2.46                     | 0.50              |
| 1:1A:2634:C:H2'    | 1:1A:2635:U:C6    | 2.47                     | 0.50              |
| 1:1A:2639:U:O2'    | 35:2a:26:PRO:HG3  | 2.12                     | 0.50              |
| 1:1A:3795:A:H2'    | 1:1A:3796:U:C6    | 2.46                     | 0.50              |
| 1:1A:4043:G:H5''   | 1:1A:4045:G:H21   | 1.76                     | 0.50              |
| 1:1A:4098:A:H2'    | 1:1A:4099:G:C5'   | 2.42                     | 0.50              |
| 1:1A:4566:U:H2'    | 1:1A:4567:G:O4'   | 2.11                     | 0.50              |
| 1:1A:4578:G:O2'    | 1:1A:4579:U:H5'   | 2.11                     | 0.50              |
| 1:1A:4764:A:H62    | 15:2G:4:ARG:HH12  | 1.59                     | 0.50              |
| 1:1A:4915:G:H2'    | 1:1A:4916:G:H8    | 1.77                     | 0.50              |
| 1:1A:4928:C:O2     | 15:2G:118:MET:HE1 | 2.12                     | 0.50              |
| 6:1F:193:LYS:HD2   | 6:1F:196:MET:HE3  | 1.93                     | 0.50              |
| 8:1H:138:ARG:HH11  | 8:1H:170:SER:HA   | 1.76                     | 0.50              |
| 13:2E:24:ILE:HG12  | 13:2E:128:LEU:CB  | 2.41                     | 0.50              |
| 25:2Q:104:GLN:HA   | 25:2Q:107:GLN:CD  | 2.37                     | 0.50              |
| 27:2S:82:ILE:CG2   | 27:2S:83:GLU:H    | 2.24                     | 0.50              |
| 47:2m:808:A:H2'    | 47:2m:809:A:O4'   | 2.12                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1535:U:H5''  | 47:2m:1536:G:C8    | 2.47                     | 0.50              |
| 48:2n:11:LYS:HA    | 48:2n:11:LYS:HE3   | 1.94                     | 0.50              |
| 50:2p:175:VAL:CG2  | 50:2p:184:ILE:HD11 | 2.42                     | 0.50              |
| 51:2q:163:ASP:OD1  | 51:2q:163:ASP:N    | 2.39                     | 0.50              |
| 57:2w:94:VAL:O     | 57:2w:105:VAL:HG22 | 2.12                     | 0.50              |
| 58:2x:133:GLY:C    | 58:2x:140:ARG:HD2  | 2.37                     | 0.50              |
| 59:2y:98:VAL:O     | 59:2y:120:THR:N    | 2.38                     | 0.50              |
| 61:20:113:VAL:HG23 | 61:20:122:LYS:O    | 2.12                     | 0.50              |
| 69:3G:144:SER:HB3  | 69:3G:150:ALA:HB2  | 1.93                     | 0.50              |
| 75:3M:106:THR:HG22 | 75:3M:123:GLY:HA3  | 1.93                     | 0.50              |
| 76:3N:27:VAL:HB    | 76:3N:69:THR:HG23  | 1.94                     | 0.50              |
| 1:1A:178:C:H2'     | 1:1A:179:G:H8      | 1.77                     | 0.49              |
| 1:1A:280:G:C5'     | 16:2H:14:LYS:HE2   | 2.35                     | 0.49              |
| 1:1A:457:G:H2'     | 1:1A:458:C:H6      | 1.76                     | 0.49              |
| 1:1A:1172:C:O2     | 1:1A:1172:C:H3'    | 2.12                     | 0.49              |
| 1:1A:4236:G:H4'    | 1:1A:4328:G:O2'    | 2.12                     | 0.49              |
| 4:1D:207:VAL:HG13  | 4:1D:208:GLU:HG3   | 1.93                     | 0.49              |
| 7:1G:55:VAL:HG13   | 7:1G:60:ILE:HD13   | 1.92                     | 0.49              |
| 10:2B:50:ASP:HB2   | 26:2R:40:ILE:HG12  | 1.94                     | 0.49              |
| 25:2Q:73:ARG:HH22  | 70:3H:114:VAL:CG2  | 2.25                     | 0.49              |
| 28:2T:103:ASP:OD1  | 28:2T:103:ASP:C    | 2.55                     | 0.49              |
| 46:2l:113:SER:HB3  | 46:2l:116:LEU:HD21 | 1.93                     | 0.49              |
| 47:2m:67:C:O2'     | 70:3H:164:LYS:NZ   | 2.38                     | 0.49              |
| 47:2m:113:G:N2     | 47:2m:293:C:O5'    | 2.45                     | 0.49              |
| 47:2m:1464:C:H5''  | 47:2m:1465:A:P     | 2.52                     | 0.49              |
| 48:2n:124:VAL:CG1  | 48:2n:130:ASP:HB2  | 2.42                     | 0.49              |
| 50:2p:106:ARG:HG3  | 50:2p:175:VAL:CG2  | 2.34                     | 0.49              |
| 51:2q:7:LYS:O      | 51:2q:30:ARG:HG2   | 2.12                     | 0.49              |
| 54:2t:46:VAL:CG1   | 54:2t:54:LYS:HG3   | 2.42                     | 0.49              |
| 56:2v:61:PRO:HA    | 56:2v:66:VAL:CG2   | 2.42                     | 0.49              |
| 58:2x:137:ALA:O    | 58:2x:140:ARG:NH1  | 2.45                     | 0.49              |
| 60:2z:5:ILE:CD1    | 77:3O:49:LEU:HB3   | 2.33                     | 0.49              |
| 62:21:21:ARG:HB3   | 62:21:115:THR:HG21 | 1.94                     | 0.49              |
| 63:3A:55:ILE:HG22  | 63:3A:60:ARG:HG3   | 1.94                     | 0.49              |
| 66:3D:11:LEU:CD1   | 66:3D:55:VAL:HG22  | 2.42                     | 0.49              |
| 68:3F:290:ALA:O    | 68:3F:298:LEU:HD23 | 2.12                     | 0.49              |
| 69:3G:103:LYS:C    | 69:3G:130:ILE:HD12 | 2.37                     | 0.49              |
| 69:3G:270:THR:O    | 69:3G:274:VAL:HG13 | 2.11                     | 0.49              |
| 72:3J:17:ALA:HA    | 72:3J:20:GLU:CG    | 2.42                     | 0.49              |
| 74:3L:85:CYS:HB2   | 74:3L:124:MET:HE3  | 1.94                     | 0.49              |
| 76:3N:25:ILE:HG12  | 76:3N:44:LEU:HD11  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:65:A:N1      | 1:1A:76:A:H5''     | 2.26                     | 0.49              |
| 1:1A:227:A:N6     | 1:1A:241:G:H2'     | 2.28                     | 0.49              |
| 1:1A:268:G:H2'    | 1:1A:269:G:H8      | 1.77                     | 0.49              |
| 1:1A:725:G:O2'    | 1:1A:726:G:H5'     | 2.11                     | 0.49              |
| 1:1A:1173:G:H3'   | 1:1A:1174:G:C8     | 2.47                     | 0.49              |
| 1:1A:1385:G:O2'   | 1:1A:1386:C:H5'    | 2.12                     | 0.49              |
| 1:1A:1871:A:O2'   | 1:1A:1872:G:H5'    | 2.11                     | 0.49              |
| 1:1A:2101:C:H2'   | 1:1A:2102:G:C8     | 2.46                     | 0.49              |
| 1:1A:2358:G:H2'   | 1:1A:2359:U:O4'    | 2.12                     | 0.49              |
| 1:1A:2639:U:H1'   | 35:2a:26:PRO:HA    | 1.94                     | 0.49              |
| 1:1A:2747:U:H2'   | 1:1A:2748:C:C6     | 2.46                     | 0.49              |
| 1:1A:4043:G:H5''  | 1:1A:4045:G:N2     | 2.27                     | 0.49              |
| 1:1A:4970:C:C2    | 1:1A:4971:A:C8     | 3.00                     | 0.49              |
| 2:1B:55:A:H4'     | 13:2E:155:HIS:HB2  | 1.94                     | 0.49              |
| 4:1D:103:PRO:HG2  | 4:1D:106:THR:CG2   | 2.41                     | 0.49              |
| 9:2A:24:ASN:O     | 9:2A:28:LEU:HD11   | 2.12                     | 0.49              |
| 10:2B:94:GLN:HG2  | 10:2B:218:LEU:HD21 | 1.94                     | 0.49              |
| 21:2M:45:TRP:NE1  | 21:2M:56:LYS:HG3   | 2.27                     | 0.49              |
| 38:2d:20:ARG:NH2  | 38:2d:39:TYR:OH    | 2.45                     | 0.49              |
| 47:2m:444:G:O6    | 54:2t:26:LYS:HE2   | 2.11                     | 0.49              |
| 47:2m:606:G:N3    | 47:2m:606:G:H2'    | 2.27                     | 0.49              |
| 47:2m:886:A:H2    | 47:2m:901:G:H1'    | 1.75                     | 0.49              |
| 49:2o:62:LEU:HA   | 49:2o:65:ARG:NE    | 2.28                     | 0.49              |
| 65:3C:52:ASP:OD1  | 74:3L:121:ARG:HD3  | 2.12                     | 0.49              |
| 70:3H:18:VAL:HG11 | 70:3H:24:LEU:CD2   | 2.37                     | 0.49              |
| 71:3I:69:ARG:O    | 71:3I:73:GLU:HG3   | 2.11                     | 0.49              |
| 72:3J:49:LEU:O    | 72:3J:111:VAL:HG22 | 2.12                     | 0.49              |
| 72:3J:64:LEU:HD11 | 80:3R:106:TYR:CD2  | 2.47                     | 0.49              |
| 77:3O:49:LEU:H    | 77:3O:83:LEU:HD11  | 1.76                     | 0.49              |
| 78:3P:33:MET:HE3  | 78:3P:79:PHE:CD1   | 2.41                     | 0.49              |
| 1:1A:173:C:H5'    | 14:2F:129:ARG:NH2  | 2.27                     | 0.49              |
| 1:1A:294:G:O6     | 1:1A:315:G:H1'     | 2.12                     | 0.49              |
| 1:1A:1074:G:H3'   | 1:1A:1075:G:H8     | 1.75                     | 0.49              |
| 1:1A:1241:C:H2'   | 1:1A:1242:G:C1'    | 2.43                     | 0.49              |
| 1:1A:2045:G:O2'   | 1:1A:2046:G:H5''   | 2.12                     | 0.49              |
| 1:1A:2684:C:O2'   | 1:1A:2685:C:H5'    | 2.13                     | 0.49              |
| 1:1A:2756:G:O2'   | 1:1A:2757:A:H5'    | 2.11                     | 0.49              |
| 1:1A:3753:G:H1    | 1:1A:3770:U:H3     | 1.60                     | 0.49              |
| 1:1A:4208:U:H2'   | 1:1A:4209:G:H8     | 1.78                     | 0.49              |
| 1:1A:4343:U:H2'   | 1:1A:4344:U:C6     | 2.48                     | 0.49              |
| 1:1A:4563:U:C2    | 1:1A:4564:A:C8     | 3.01                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:4578:G:H2'    | 1:1A:4579:U:C6    | 2.47                     | 0.49              |
| 1:1A:4765:G:N2     | 1:1A:4869:U:H3    | 2.08                     | 0.49              |
| 6:1F:66:SER:O      | 6:1F:67:TRP:HB2   | 2.11                     | 0.49              |
| 9:2A:32:ARG:O      | 9:2A:36:LYS:HG2   | 2.11                     | 0.49              |
| 11:2C:16:VAL:HG11  | 11:2C:85:THR:HG23 | 1.93                     | 0.49              |
| 17:2I:74:ARG:O     | 17:2I:142:ALA:HB1 | 2.13                     | 0.49              |
| 21:2M:37:HIS:O     | 21:2M:41:LYS:HG3  | 2.11                     | 0.49              |
| 24:2P:85:ARG:HG2   | 24:2P:85:ARG:HH11 | 1.78                     | 0.49              |
| 29:2U:93:ASN:OD1   | 29:2U:95:THR:N    | 2.46                     | 0.49              |
| 45:2k:82:ILE:CG2   | 45:2k:89:THR:HG23 | 2.41                     | 0.49              |
| 46:2l:105:LYS:HD2  | 46:2l:105:LYS:N   | 2.27                     | 0.49              |
| 47:2m:106:C:H2'    | 47:2m:107:A:H8    | 1.77                     | 0.49              |
| 47:2m:480:G:H2'    | 47:2m:481:C:C6    | 2.47                     | 0.49              |
| 47:2m:947:G:H2'    | 47:2m:948:C:C6    | 2.47                     | 0.49              |
| 47:2m:1062:A:H2'   | 47:2m:1063:C:C6   | 2.47                     | 0.49              |
| 47:2m:1421:A:H5''  | 47:2m:1422:G:N3   | 2.28                     | 0.49              |
| 47:2m:1779:G:H5''  | 47:2m:1780:G:OP2  | 2.12                     | 0.49              |
| 48:2n:63:ARG:CG    | 48:2n:185:MET:HE1 | 2.41                     | 0.49              |
| 49:2o:143:THR:HG22 | 49:2o:205:TYR:CD1 | 2.47                     | 0.49              |
| 53:2s:169:LYS:HG2  | 53:2s:173:PHE:CE1 | 2.47                     | 0.49              |
| 54:2t:3:ILE:HD12   | 54:2t:4:SER:N     | 2.28                     | 0.49              |
| 57:2w:17:TYR:CE2   | 57:2w:18:ARG:HG3  | 2.47                     | 0.49              |
| 57:2w:25:LEU:HD11  | 57:2w:87:PRO:HG2  | 1.94                     | 0.49              |
| 57:2w:34:MET:HE2   | 57:2w:42:ARG:HA   | 1.95                     | 0.49              |
| 59:2y:33:ARG:HA    | 59:2y:36:GLU:HG3  | 1.93                     | 0.49              |
| 60:2z:36:VAL:HG21  | 60:2z:71:MET:SD   | 2.52                     | 0.49              |
| 60:2z:44:VAL:HB    | 60:2z:70:ILE:HD13 | 1.94                     | 0.49              |
| 60:2z:98:VAL:HG21  | 60:2z:103:LEU:HA  | 1.94                     | 0.49              |
| 68:3F:153:CYS:SG   | 68:3F:155:ARG:NE  | 2.85                     | 0.49              |
| 68:3F:158:PRO:HG3  | 68:3F:200:VAL:CG2 | 2.42                     | 0.49              |
| 71:3I:140:GLN:HG3  | 71:3I:141:VAL:N   | 2.27                     | 0.49              |
| 1:1A:56:A:O2'      | 1:1A:57:G:H5'     | 2.12                     | 0.49              |
| 1:1A:135:G:N2      | 36:2b:96:ASN:HA   | 2.27                     | 0.49              |
| 1:1A:317:A:C2      | 1:1A:4361:U:H1'   | 2.46                     | 0.49              |
| 1:1A:1175:A:O2'    | 1:1A:1176:C:H5'   | 2.12                     | 0.49              |
| 1:1A:1296:G:O2'    | 1:1A:1297:U:O5'   | 2.27                     | 0.49              |
| 1:1A:1297:U:OP1    | 34:2Z:56:ASN:HB2  | 2.13                     | 0.49              |
| 1:1A:1346:C:H2'    | 1:1A:1347:G:C8    | 2.47                     | 0.49              |
| 1:1A:1521:C:C2'    | 1:1A:1522:G:H5'   | 2.42                     | 0.49              |
| 1:1A:1786:A:H2'    | 1:1A:1789:C:C5    | 2.47                     | 0.49              |
| 1:1A:2534:C:O2'    | 1:1A:2535:G:H5'   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:3760:A:H3'   | 1:1A:3761:C:H5'    | 1.94                     | 0.49              |
| 1:1A:3969:G:N2    | 1:1A:4053:A:OP1    | 2.45                     | 0.49              |
| 1:1A:3971:G:OP1   | 46:2l:28:PHE:HE2   | 1.95                     | 0.49              |
| 1:1A:4466:C:H2'   | 1:1A:4467:A:H8     | 1.76                     | 0.49              |
| 1:1A:4769:G:H2'   | 1:1A:4770:U:H5''   | 1.94                     | 0.49              |
| 1:1A:4915:G:H2'   | 1:1A:4916:G:C8     | 2.47                     | 0.49              |
| 5:1E:217:ILE:HD12 | 5:1E:347:LEU:HB3   | 1.94                     | 0.49              |
| 6:1F:63:SER:O     | 6:1F:63:SER:OG     | 2.25                     | 0.49              |
| 27:2S:44:VAL:HG13 | 27:2S:122:LYS:HD3  | 1.93                     | 0.49              |
| 29:2U:95:THR:OG1  | 29:2U:96:GLY:N     | 2.46                     | 0.49              |
| 39:2e:33:LYS:HG2  | 39:2e:46:VAL:HG22  | 1.94                     | 0.49              |
| 46:2l:71:GLN:HA   | 46:2l:84:HIS:CE1   | 2.47                     | 0.49              |
| 47:2m:96:C:O2'    | 47:2m:97:U:H5'     | 2.13                     | 0.49              |
| 47:2m:153:G:H21   | 70:3H:13:GLN:CD    | 2.21                     | 0.49              |
| 47:2m:356:C:O2    | 47:2m:356:C:C2'    | 2.60                     | 0.49              |
| 47:2m:379:C:P     | 54:2t:181:GLN:HE21 | 2.35                     | 0.49              |
| 47:2m:510:G:C2'   | 47:2m:511:U:H5'    | 2.43                     | 0.49              |
| 47:2m:671:A:H4'   | 47:2m:672:A:OP1    | 2.12                     | 0.49              |
| 47:2m:1256:G:O6   | 67:3E:31:ILE:HD11  | 2.12                     | 0.49              |
| 47:2m:1316:C:H2'  | 47:2m:1317:C:O4'   | 2.11                     | 0.49              |
| 47:2m:1434:C:O2   | 47:2m:1435:C:N4    | 2.46                     | 0.49              |
| 49:2o:174:ARG:O   | 49:2o:178:THR:OG1  | 2.27                     | 0.49              |
| 50:2p:29:LEU:HD23 | 50:2p:58:VAL:HG23  | 1.94                     | 0.49              |
| 50:2p:76:ARG:HD3  | 55:2u:68:TYR:OH    | 2.13                     | 0.49              |
| 58:2x:44:PRO:HA   | 58:2x:45:ARG:NH1   | 2.26                     | 0.49              |
| 58:2x:96:TYR:HD1  | 58:2x:100:VAL:HG21 | 1.78                     | 0.49              |
| 62:21:25:THR:HG23 | 62:21:111:GLU:HB2  | 1.95                     | 0.49              |
| 72:3J:68:LEU:CA   | 80:3R:114:ILE:HD11 | 2.37                     | 0.49              |
| 1:1A:320:C:O2'    | 1:1A:321:U:H5'     | 2.11                     | 0.49              |
| 1:1A:418:A:H5'    | 1:1A:2310:C:O2'    | 2.12                     | 0.49              |
| 1:1A:513:U:H3'    | 1:1A:514:U:C4'     | 2.40                     | 0.49              |
| 1:1A:1886:G:O2'   | 1:1A:1887:G:H5'    | 2.12                     | 0.49              |
| 1:1A:2455:G:H1'   | 1:1A:2471:G:C2     | 2.47                     | 0.49              |
| 1:1A:2489:C:H4'   | 1:1A:2491:C:H42    | 1.76                     | 0.49              |
| 1:1A:2699:C:O2'   | 1:1A:2700:G:H5'    | 2.12                     | 0.49              |
| 1:1A:2893:U:H2'   | 1:1A:2894:A:H8     | 1.77                     | 0.49              |
| 1:1A:2903:G:H5''  | 1:1A:2904:U:H5     | 1.78                     | 0.49              |
| 1:1A:3621:A:C8    | 1:1A:4642:U:H1'    | 2.47                     | 0.49              |
| 1:1A:3727:A:H2'   | 1:1A:3728:A:C8     | 2.48                     | 0.49              |
| 1:1A:4060:U:O2'   | 1:1A:4061:G:P      | 2.70                     | 0.49              |
| 1:1A:4156:G:OP1   | 1:1A:4158:C:H5'    | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4422:A:C2'   | 1:1A:4423:U:H5'    | 2.43                     | 0.49              |
| 1:1A:4452:U:O2'   | 1:1A:4453:C:OP1    | 2.23                     | 0.49              |
| 14:2F:111:GLN:OE1 | 14:2F:111:GLN:HA   | 2.11                     | 0.49              |
| 20:2L:183:GLU:CA  | 20:2L:186:LYS:HE3  | 2.26                     | 0.49              |
| 27:2S:69:LYS:HZ3  | 27:2S:69:LYS:HB2   | 1.76                     | 0.49              |
| 28:2T:28:ASN:HB2  | 28:2T:77:TYR:OH    | 2.13                     | 0.49              |
| 33:2Y:119:ALA:HB2 | 45:2k:119:ARG:NH2  | 2.28                     | 0.49              |
| 35:2a:107:LEU:HA  | 35:2a:110:GLN:NE2  | 2.26                     | 0.49              |
| 44:2j:38:THR:HA   | 44:2j:45:THR:HA    | 1.93                     | 0.49              |
| 45:2k:7:TRP:O     | 45:2k:11:ARG:HB2   | 2.11                     | 0.49              |
| 46:2l:65:VAL:O    | 46:2l:111:LEU:HD13 | 2.13                     | 0.49              |
| 47:2m:314:U:OP1   | 70:3H:191:ARG:NH2  | 2.45                     | 0.49              |
| 47:2m:429:C:OP1   | 51:2q:10:LYS:NZ    | 2.35                     | 0.49              |
| 47:2m:1194:A:H1'  | 47:2m:1195:A:O4'   | 2.13                     | 0.49              |
| 47:2m:1333:U:OP1  | 50:2p:146:ARG:HA   | 2.13                     | 0.49              |
| 47:2m:1759:G:N2   | 47:2m:1774:C:OP1   | 2.43                     | 0.49              |
| 48:2n:205:ARG:HB3 | 48:2n:210:ILE:HD11 | 1.92                     | 0.49              |
| 49:2o:103:MET:HG2 | 49:2o:104:ASP:N    | 2.27                     | 0.49              |
| 50:2p:92:ALA:CB   | 50:2p:198:ILE:HD11 | 2.43                     | 0.49              |
| 50:2p:158:ILE:O   | 50:2p:164:VAL:HG11 | 2.12                     | 0.49              |
| 52:2r:29:GLN:C    | 52:2r:30:ILE:HD13  | 2.36                     | 0.49              |
| 52:2r:40:ALA:HB1  | 52:2r:67:PRO:HA    | 1.93                     | 0.49              |
| 52:2r:150:ALA:O   | 52:2r:154:LEU:HD13 | 2.13                     | 0.49              |
| 52:2r:174:ALA:O   | 52:2r:178:ILE:HG12 | 2.13                     | 0.49              |
| 53:2s:58:LYS:CG   | 53:2s:90:LYS:HD2   | 2.41                     | 0.49              |
| 54:2t:84:ASN:HD21 | 54:2t:97:VAL:HG21  | 1.77                     | 0.49              |
| 55:2u:32:HIS:CE1  | 55:2u:45:VAL:HG21  | 2.46                     | 0.49              |
| 56:2v:23:VAL:HB   | 56:2v:25:LEU:CD2   | 2.43                     | 0.49              |
| 57:2w:28:MET:HG2  | 57:2w:32:GLN:HG3   | 1.95                     | 0.49              |
| 57:2w:75:VAL:HG22 | 57:2w:93:MET:HG2   | 1.93                     | 0.49              |
| 58:2x:42:ILE:HG12 | 58:2x:51:LEU:CD1   | 2.41                     | 0.49              |
| 58:2x:60:LYS:HD3  | 58:2x:60:LYS:C     | 2.37                     | 0.49              |
| 60:2z:27:ALA:HA   | 60:2z:45:LEU:HD11  | 1.94                     | 0.49              |
| 73:3K:54:LEU:HD13 | 73:3K:63:VAL:CG2   | 2.42                     | 0.49              |
| 77:3O:56:ASP:HB3  | 77:3O:60:LYS:HZ1   | 1.78                     | 0.49              |
| 1:1A:752:G:H2'    | 1:1A:753:C:C1'     | 2.43                     | 0.49              |
| 1:1A:959:G:H8     | 1:1A:959:G:OP2     | 1.95                     | 0.49              |
| 1:1A:1663:C:H1'   | 1:1A:2320:G:N2     | 2.28                     | 0.49              |
| 1:1A:2489:C:H4'   | 1:1A:2491:C:N4     | 2.27                     | 0.49              |
| 1:1A:2894:A:H2'   | 1:1A:2895:A:H8     | 1.77                     | 0.49              |
| 1:1A:3602:C:O2'   | 1:1A:3603:G:H5'    | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:3721:U:H2'    | 1:1A:3722:G:H8     | 1.78                     | 0.49              |
| 1:1A:3872:A:C2'    | 1:1A:3873:G:H5'    | 2.42                     | 0.49              |
| 1:1A:4218:U:H5''   | 1:1A:4219:A:OP1    | 2.12                     | 0.49              |
| 1:1A:4311:A:O2'    | 1:1A:4312:U:H5'    | 2.11                     | 0.49              |
| 3:1C:6:C:H2'       | 3:1C:7:U:H6        | 1.77                     | 0.49              |
| 3:1C:117:C:H4'     | 26:2R:55:ARG:HH12  | 1.78                     | 0.49              |
| 18:2J:41:ILE:HD13  | 18:2J:150:LEU:HD21 | 1.93                     | 0.49              |
| 43:2i:12:CYS:HB3   | 43:2i:15:CYS:SG    | 2.53                     | 0.49              |
| 46:2l:47:LYS:NZ    | 46:2l:159:MET:O    | 2.46                     | 0.49              |
| 47:2m:14:C:H2'     | 47:2m:15:U:C6      | 2.47                     | 0.49              |
| 47:2m:1093:A:H2'   | 47:2m:1094:C:H6    | 1.76                     | 0.49              |
| 47:2m:1189:A:H2'   | 47:2m:1190:A:H8    | 1.77                     | 0.49              |
| 47:2m:1307:U:O2    | 80:3R:135:HIS:HA   | 2.13                     | 0.49              |
| 47:2m:1762:C:P     | 47:2m:1772:C:H42   | 2.34                     | 0.49              |
| 49:2o:110:MET:HE3  | 49:2o:110:MET:O    | 2.11                     | 0.49              |
| 49:2o:187:LYS:O    | 49:2o:190:PRO:HD2  | 2.11                     | 0.49              |
| 50:2p:217:ILE:HG23 | 50:2p:218:LEU:CD2  | 2.38                     | 0.49              |
| 51:2q:137:PRO:HG2  | 51:2q:149:TYR:HA   | 1.95                     | 0.49              |
| 55:2u:41:PRO:HG2   | 55:2u:44:HIS:ND1   | 2.28                     | 0.49              |
| 57:2w:65:LYS:HE2   | 57:2w:65:LYS:N     | 2.28                     | 0.49              |
| 58:2x:11:GLN:OE1   | 58:2x:71:ARG:NH2   | 2.46                     | 0.49              |
| 59:2y:45:LYS:HE2   | 59:2y:49:LYS:HE3   | 1.95                     | 0.49              |
| 61:20:41:LYS:HD2   | 61:20:42:HIS:N     | 2.28                     | 0.49              |
| 61:20:60:THR:HG22  | 61:20:107:LEU:CD1  | 2.42                     | 0.49              |
| 61:20:114:GLU:OE1  | 61:20:124:THR:HG22 | 2.11                     | 0.49              |
| 63:3A:4:ASP:N      | 69:3G:173:LYS:O    | 2.24                     | 0.49              |
| 63:3A:59:ILE:HA    | 63:3A:62:MET:HG2   | 1.95                     | 0.49              |
| 66:3D:14:VAL:HG13  | 66:3D:52:GLU:CG    | 2.41                     | 0.49              |
| 70:3H:14:LYS:HZ3   | 70:3H:16:ILE:HB    | 1.78                     | 0.49              |
| 70:3H:147:LEU:HB3  | 70:3H:151:ASP:OD2  | 2.12                     | 0.49              |
| 71:3I:32:ILE:HD11  | 71:3I:40:LYS:CA    | 2.42                     | 0.49              |
| 71:3I:113:GLN:HG3  | 71:3I:149:VAL:HG21 | 1.94                     | 0.49              |
| 1:1A:294:G:H3'     | 1:1A:294:G:N3      | 2.27                     | 0.49              |
| 1:1A:700:G:H2'     | 1:1A:701:G:H8      | 1.78                     | 0.49              |
| 1:1A:743:G:H2'     | 1:1A:744:G:C1'     | 2.42                     | 0.49              |
| 1:1A:1329:G:C2     | 1:1A:3865:A:H1'    | 2.48                     | 0.49              |
| 1:1A:1461:C:H2'    | 1:1A:1462:A:C8     | 2.47                     | 0.49              |
| 1:1A:1533:A:N1     | 1:1A:1636:U:H1'    | 2.26                     | 0.49              |
| 1:1A:2675:G:HO2'   | 1:1A:2676:A:P      | 2.35                     | 0.49              |
| 1:1A:4327:C:C2'    | 1:1A:4328:G:H5'    | 2.42                     | 0.49              |
| 1:1A:4376:A:H5''   | 1:1A:4377:G:O5'    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4384:U:O2'   | 1:1A:4386:C:OP1    | 2.26                     | 0.49              |
| 1:1A:4884:G:N2    | 1:1A:4936:G:H22    | 2.11                     | 0.49              |
| 3:1C:123:U:H5     | 3:1C:124:U:H1'     | 1.76                     | 0.49              |
| 7:1G:212:MET:HE1  | 7:1G:233:PRO:CD    | 2.42                     | 0.49              |
| 10:2B:232:GLU:CD  | 10:2B:232:GLU:H    | 2.21                     | 0.49              |
| 13:2E:22:LEU:HD21 | 13:2E:130:PHE:CD2  | 2.48                     | 0.49              |
| 23:2O:37:ALA:O    | 23:2O:41:GLN:HG2   | 2.12                     | 0.49              |
| 24:2P:42:VAL:HG13 | 24:2P:61:VAL:HG12  | 1.94                     | 0.49              |
| 39:2e:5:ILE:CD1   | 39:2e:43:TYR:HB3   | 2.41                     | 0.49              |
| 47:2m:414:A:O2'   | 47:2m:415:A:H5'    | 2.12                     | 0.49              |
| 47:2m:420:G:O2'   | 47:2m:660:C:N3     | 2.44                     | 0.49              |
| 47:2m:674:C:H2'   | 47:2m:675:U:H6     | 1.73                     | 0.49              |
| 47:2m:849:A:O2'   | 47:2m:850:C:H5'    | 2.12                     | 0.49              |
| 47:2m:1204:A:O2'  | 47:2m:1205:C:H5'   | 2.12                     | 0.49              |
| 47:2m:1276:A:H5'  | 47:2m:1277:C:OP2   | 2.12                     | 0.49              |
| 47:2m:1313:A:OP2  | 72:3J:33:ARG:HD2   | 2.13                     | 0.49              |
| 47:2m:1567:G:OP2  | 61:20:33:TRP:HZ3   | 1.94                     | 0.49              |
| 47:2m:1571:G:H2'  | 47:2m:1572:C:H6    | 1.75                     | 0.49              |
| 48:2n:62:ALA:HA   | 48:2n:65:ILE:HG22  | 1.93                     | 0.49              |
| 50:2p:69:LEU:HD23 | 50:2p:69:LEU:O     | 2.13                     | 0.49              |
| 52:2r:34:SER:OG   | 66:3D:11:LEU:HD11  | 2.12                     | 0.49              |
| 54:2t:145:ILE:C   | 54:2t:145:ILE:HD12 | 2.37                     | 0.49              |
| 56:2v:23:VAL:HB   | 56:2v:25:LEU:HD22  | 1.93                     | 0.49              |
| 56:2v:136:LYS:HD3 | 56:2v:137:THR:HG23 | 1.94                     | 0.49              |
| 58:2x:8:GLN:HG2   | 58:2x:27:ARG:NH1   | 2.27                     | 0.49              |
| 58:2x:118:THR:HA  | 58:2x:121:VAL:HG22 | 1.95                     | 0.49              |
| 64:3B:56:GLY:HA3  | 79:3Q:3:HIS:CE1    | 2.48                     | 0.49              |
| 69:3G:167:ARG:HG2 | 69:3G:219:ILE:CD1  | 2.43                     | 0.49              |
| 70:3H:7:PHE:CE2   | 70:3H:9:ALA:HB3    | 2.48                     | 0.49              |
| 71:3I:24:ARG:NH1  | 71:3I:28:GLU:OE2   | 2.45                     | 0.49              |
| 1:1A:320:C:C2'    | 1:1A:321:U:H5'     | 2.43                     | 0.49              |
| 1:1A:384:A:OP2    | 81:1A:5106:84D:N   | 2.46                     | 0.49              |
| 1:1A:1345:A:H2'   | 1:1A:1346:C:H6     | 1.76                     | 0.49              |
| 1:1A:1362:G:O2'   | 1:1A:1363:C:H5'    | 2.12                     | 0.49              |
| 1:1A:2261:G:H4'   | 8:1H:112:MET:CE    | 2.43                     | 0.49              |
| 1:1A:2673:G:H5''  | 1:1A:2675:G:O4'    | 2.13                     | 0.49              |
| 1:1A:4260:U:H4'   | 13:2E:21:CYS:SG    | 2.52                     | 0.49              |
| 1:1A:4307:A:H4'   | 19:2K:186:TYR:CG   | 2.47                     | 0.49              |
| 1:1A:4745:G:N2    | 1:1A:4954:G:H1     | 2.07                     | 0.49              |
| 1:1A:4988:U:HO2'  | 1:1A:4989:U:P      | 2.33                     | 0.49              |
| 4:1D:101:VAL:C    | 4:1D:102:LEU:HD23  | 2.37                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:2E:121:PRO:HA  | 60:2z:11:HIS:ND1   | 2.28                     | 0.49              |
| 14:2F:128:PRO:HB3 | 14:2F:134:PRO:HA   | 1.95                     | 0.49              |
| 23:2O:91:LEU:HD13 | 23:2O:96:LEU:HB3   | 1.95                     | 0.49              |
| 28:2T:10:VAL:HG23 | 28:2T:87:VAL:HG12  | 1.94                     | 0.49              |
| 46:2l:66:CYS:CB   | 46:2l:82:ILE:HD13  | 2.39                     | 0.49              |
| 47:2m:77:A:H2     | 70:3H:175:LYS:HD3  | 1.76                     | 0.49              |
| 47:2m:570:C:H2'   | 47:2m:571:U:H6     | 1.77                     | 0.49              |
| 47:2m:1239:U:O2'  | 47:2m:1241:A:N7    | 2.37                     | 0.49              |
| 52:2r:122:ARG:NH1 | 52:2r:146:ARG:HH22 | 2.11                     | 0.49              |
| 53:2s:75:ILE:HG13 | 53:2s:79:LEU:CD1   | 2.43                     | 0.49              |
| 58:2x:107:GLU:HA  | 58:2x:110:ASP:OD2  | 2.13                     | 0.49              |
| 60:2z:44:VAL:HB   | 60:2z:70:ILE:HD12  | 1.94                     | 0.49              |
| 60:2z:117:ILE:O   | 60:2z:118:ARG:HB3  | 2.12                     | 0.49              |
| 70:3H:30:LYS:HD3  | 70:3H:36:VAL:CG2   | 2.37                     | 0.49              |
| 72:3J:65:VAL:HG22 | 72:3J:69:LEU:CD1   | 2.43                     | 0.49              |
| 73:3K:38:TYR:CZ   | 73:3K:78:LYS:HD2   | 2.48                     | 0.49              |
| 74:3L:84:ARG:NH1  | 74:3L:87:GLU:OE2   | 2.46                     | 0.49              |
| 74:3L:85:CYS:HB2  | 74:3L:124:MET:HE1  | 1.95                     | 0.49              |
| 76:3N:20:ARG:HB3  | 76:3N:76:TYR:CD1   | 2.48                     | 0.49              |
| 1:1A:35:U:H5'     | 1:1A:36:U:OP2      | 2.12                     | 0.49              |
| 1:1A:677:G:H2'    | 1:1A:678:C:C6      | 2.48                     | 0.49              |
| 1:1A:1666:C:O2'   | 1:1A:1688:G:OP1    | 2.25                     | 0.49              |
| 1:1A:1817:U:C2'   | 1:1A:1818:G:H5'    | 2.43                     | 0.49              |
| 1:1A:1971:C:H42   | 1:1A:2001:G:P      | 2.35                     | 0.49              |
| 1:1A:2080:U:H2'   | 1:1A:2081:C:C6     | 2.47                     | 0.49              |
| 1:1A:2715:G:O2'   | 1:1A:2716:C:H5'    | 2.12                     | 0.49              |
| 1:1A:3612:C:O4'   | 1:1A:5016:A:H1'    | 2.13                     | 0.49              |
| 1:1A:4606:G:O2'   | 1:1A:4607:A:H5'    | 2.12                     | 0.49              |
| 1:1A:4731:G:H1'   | 1:1A:4732:G:OP2    | 2.13                     | 0.49              |
| 1:1A:4924:C:O2'   | 1:1A:4925:U:O4'    | 2.31                     | 0.49              |
| 3:1C:16:G:HO2'    | 3:1C:17:A:P        | 2.35                     | 0.49              |
| 3:1C:84:A:H4'     | 3:1C:85:U:H4'      | 1.95                     | 0.49              |
| 5:1E:397:ILE:O    | 5:1E:401:GLU:HG2   | 2.12                     | 0.49              |
| 11:2C:44:GLU:HG3  | 15:2G:2:VAL:CG2    | 2.43                     | 0.49              |
| 13:2E:58:ARG:O    | 13:2E:58:ARG:HG3   | 2.13                     | 0.49              |
| 17:2I:185:VAL:O   | 17:2I:185:VAL:CG2  | 2.60                     | 0.49              |
| 22:2N:26:PRO:O    | 22:2N:29:THR:HG23  | 2.13                     | 0.49              |
| 23:2O:20:LYS:H    | 23:2O:73:THR:HA    | 1.78                     | 0.49              |
| 35:2a:107:LEU:CD1 | 35:2a:110:GLN:HE21 | 2.19                     | 0.49              |
| 41:2g:94:MET:O    | 41:2g:95:ILE:HD13  | 2.12                     | 0.49              |
| 47:2m:120:U:H1'   | 51:2q:33:THR:O     | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:803:C:H2'    | 47:2m:804:U:C6     | 2.48                     | 0.49              |
| 47:2m:844:U:P      | 51:2q:240:ARG:HH22 | 2.35                     | 0.49              |
| 47:2m:901:G:C2     | 47:2m:902:G:H1'    | 2.47                     | 0.49              |
| 47:2m:972:A:H3'    | 47:2m:973:C:H6     | 1.78                     | 0.49              |
| 47:2m:1253:A:H4'   | 47:2m:1254:C:H5''  | 1.95                     | 0.49              |
| 47:2m:1452:A:H5'   | 47:2m:1453:C:C5    | 2.48                     | 0.49              |
| 47:2m:1839:U:H1'   | 47:2m:1863:A:C2    | 2.47                     | 0.49              |
| 48:2n:23:THR:HG1   | 48:2n:170:SER:HG   | 1.29                     | 0.49              |
| 48:2n:23:THR:CG2   | 48:2n:163:CYS:HB2  | 2.37                     | 0.49              |
| 50:2p:95:GLY:HA3   | 50:2p:125:PHE:HE1  | 1.77                     | 0.49              |
| 52:2r:186:ASN:HA   | 52:2r:191:LYS:NZ   | 2.28                     | 0.49              |
| 53:2s:147:LYS:NZ   | 53:2s:153:LEU:HB2  | 2.28                     | 0.49              |
| 56:2v:80:MET:HE1   | 56:2v:120:VAL:O    | 2.13                     | 0.49              |
| 61:20:115:LYS:CG   | 61:20:121:ARG:HG2  | 2.42                     | 0.49              |
| 62:21:62:ARG:HG2   | 62:21:81:GLN:HB2   | 1.94                     | 0.49              |
| 64:3B:115:ILE:HG22 | 64:3B:118:VAL:HB   | 1.95                     | 0.49              |
| 71:3I:81:LEU:HD22  | 71:3I:86:VAL:CG2   | 2.42                     | 0.49              |
| 72:3J:35:ILE:HA    | 72:3J:38:ALA:CB    | 2.37                     | 0.49              |
| 72:3J:50:CYS:SG    | 72:3J:69:LEU:HD13  | 2.52                     | 0.49              |
| 75:3M:117:ARG:NH1  | 75:3M:117:ARG:HB2  | 2.28                     | 0.49              |
| 1:1A:408:A:O2'     | 1:1A:411:G:OP2     | 2.24                     | 0.49              |
| 1:1A:745:G:H2'     | 1:1A:746:A:O4'     | 2.13                     | 0.49              |
| 1:1A:929:A:H2'     | 1:1A:930:G:O4'     | 2.13                     | 0.49              |
| 1:1A:966:A:H2      | 1:1A:2093:A:H2     | 1.60                     | 0.49              |
| 1:1A:1081:C:H1'    | 1:1A:1219:G:N1     | 2.27                     | 0.49              |
| 1:1A:1552:G:O2'    | 1:1A:1553:A:OP2    | 2.30                     | 0.49              |
| 1:1A:1587:G:O2'    | 1:1A:1588:U:OP2    | 2.29                     | 0.49              |
| 1:1A:2639:U:H2'    | 1:1A:2694:G:N1     | 2.27                     | 0.49              |
| 1:1A:3855:C:H2'    | 1:1A:3856:A:H8     | 1.77                     | 0.49              |
| 1:1A:4184:G:H5'    | 4:1D:233:ARG:HB2   | 1.94                     | 0.49              |
| 1:1A:4256:A:H5'    | 1:1A:4257:A:OP2    | 2.12                     | 0.49              |
| 1:1A:4635:A:H3'    | 1:1A:4636:U:H4'    | 1.95                     | 0.49              |
| 6:1F:268:ARG:HH11  | 6:1F:268:ARG:CG    | 2.26                     | 0.49              |
| 11:2C:15:ASN:OD1   | 11:2C:15:ASN:N     | 2.45                     | 0.49              |
| 18:2J:4:TYR:CE1    | 18:2J:16:LYS:HD3   | 2.48                     | 0.49              |
| 20:2L:21:LYS:HE3   | 20:2L:55:VAL:HA    | 1.94                     | 0.49              |
| 21:2M:5:GLY:O      | 21:2M:111:ARG:NH2  | 2.46                     | 0.49              |
| 21:2M:5:GLY:H      | 21:2M:111:ARG:HH22 | 1.61                     | 0.49              |
| 47:2m:514:U:C2'    | 47:2m:515:G:H5'    | 2.43                     | 0.49              |
| 47:2m:527:C:H4'    | 71:3I:121:LYS:NZ   | 2.28                     | 0.49              |
| 47:2m:1598:G:H2'   | 77:3O:80:ARG:HG2   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1676:U:H2'   | 47:2m:1677:U:O4'   | 2.13                     | 0.49              |
| 47:2m:1745:A:H2    | 47:2m:1789:G:H21   | 1.61                     | 0.49              |
| 48:2n:40:LYS:HZ1   | 59:2y:101:ASP:HB3  | 1.78                     | 0.49              |
| 48:2n:65:ILE:CG2   | 48:2n:182:VAL:HG22 | 2.43                     | 0.49              |
| 53:2s:14:GLU:O     | 53:2s:15:LYS:HB2   | 2.13                     | 0.49              |
| 53:2s:76:GLN:HB3   | 53:2s:135:PHE:CE2  | 2.47                     | 0.49              |
| 58:2x:29:ASN:N     | 58:2x:29:ASN:OD1   | 2.45                     | 0.49              |
| 59:2y:44:LYS:HD3   | 59:2y:47:ARG:NE    | 2.27                     | 0.49              |
| 61:20:18:LEU:O     | 61:20:22:LEU:HG    | 2.13                     | 0.49              |
| 71:3I:114:VAL:HG13 | 71:3I:119:LEU:HB2  | 1.94                     | 0.49              |
| 75:3M:106:THR:OG1  | 75:3M:111:MET:HE3  | 2.12                     | 0.49              |
| 1:1A:702:U:N3      | 1:1A:703:G:H1'     | 2.27                     | 0.48              |
| 1:1A:752:G:H2'     | 1:1A:753:C:O4'     | 2.13                     | 0.48              |
| 1:1A:1313:C:O2     | 1:1A:3881:G:O2'    | 2.23                     | 0.48              |
| 1:1A:2406:G:O2'    | 1:1A:2407:G:H5'    | 2.13                     | 0.48              |
| 1:1A:2544:G:O6     | 3:1C:124:U:H5'     | 2.13                     | 0.48              |
| 1:1A:3916:G:H2'    | 1:1A:3917:A:H8     | 1.78                     | 0.48              |
| 1:1A:4065:G:H2'    | 1:1A:4065:G:N3     | 2.28                     | 0.48              |
| 1:1A:4633:G:O3'    | 1:1A:4634:U:H3'    | 2.12                     | 0.48              |
| 1:1A:4913:G:H4'    | 1:1A:4914:C:O5'    | 2.12                     | 0.48              |
| 5:1E:80:GLU:OE1    | 5:1E:323:TYR:OH    | 2.19                     | 0.48              |
| 5:1E:257:TRP:O     | 5:1E:257:TRP:HE3   | 1.96                     | 0.48              |
| 24:2P:62:MET:HE3   | 24:2P:76:VAL:HG12  | 1.95                     | 0.48              |
| 37:2c:45:ARG:O     | 37:2c:45:ARG:HD3   | 2.13                     | 0.48              |
| 47:2m:575:A:OP2    | 76:3N:89:HIS:HB2   | 2.13                     | 0.48              |
| 47:2m:677:G:OP1    | 73:3K:124:ARG:HD2  | 2.13                     | 0.48              |
| 47:2m:929:G:N2     | 47:2m:1104:G:H4'   | 2.28                     | 0.48              |
| 47:2m:1261:C:H5'   | 47:2m:1262:C:OP2   | 2.13                     | 0.48              |
| 47:2m:1454:A:C8    | 59:2y:3:ARG:HD2    | 2.48                     | 0.48              |
| 47:2m:1542:C:C4'   | 61:20:11:GLN:HB3   | 2.36                     | 0.48              |
| 47:2m:1576:G:H2'   | 47:2m:1577:G:C8    | 2.48                     | 0.48              |
| 49:2o:139:CYS:HB3  | 49:2o:172:MET:HE2  | 1.95                     | 0.48              |
| 50:2p:93:THR:OG1   | 50:2p:198:ILE:HG13 | 2.12                     | 0.48              |
| 53:2s:106:ARG:HB3  | 53:2s:107:LYS:NZ   | 2.27                     | 0.48              |
| 55:2u:6:LYS:HG3    | 55:2u:7:ASN:N      | 2.28                     | 0.48              |
| 59:2y:95:ILE:C     | 59:2y:96:ILE:HD12  | 2.37                     | 0.48              |
| 64:3B:17:ARG:O     | 64:3B:21:LYS:HG3   | 2.12                     | 0.48              |
| 64:3B:32:LEU:HD11  | 64:3B:34:THR:CB    | 2.42                     | 0.48              |
| 66:3D:37:ASP:HB3   | 66:3D:40:ARG:HG2   | 1.94                     | 0.48              |
| 68:3F:77:PHE:HB3   | 68:3F:89:LEU:CD1   | 2.28                     | 0.48              |
| 70:3H:224:ARG:HG3  | 70:3H:224:ARG:NH1  | 2.28                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 71:3I:119:LEU:HD13 | 71:3I:159:PHE:CZ  | 2.47                     | 0.48              |
| 73:3K:30:SER:O     | 73:3K:34:LYS:HG3  | 2.13                     | 0.48              |
| 78:3P:36:LYS:HD3   | 78:3P:40:CYS:O    | 2.13                     | 0.48              |
| 1:1A:68:U:OP1      | 16:2H:178:HIS:ND1 | 2.33                     | 0.48              |
| 1:1A:135:G:H21     | 36:2b:96:ASN:HA   | 1.78                     | 0.48              |
| 1:1A:306:A:OP1     | 37:2c:53:TYR:HE1  | 1.95                     | 0.48              |
| 1:1A:1284:G:O2'    | 1:1A:1285:U:H5''  | 2.13                     | 0.48              |
| 1:1A:1398:A:OP1    | 29:2U:136:LYS:NZ  | 2.45                     | 0.48              |
| 1:1A:1638:A:N6     | 1:1A:2794:C:OP2   | 2.44                     | 0.48              |
| 1:1A:2323:C:H2'    | 1:1A:2324:C:C6    | 2.48                     | 0.48              |
| 1:1A:2519:U:H1'    | 1:1A:2520:C:C6    | 2.48                     | 0.48              |
| 1:1A:3653:A:C2     | 1:1A:3692:A:C4'   | 2.96                     | 0.48              |
| 1:1A:3714:G:H2'    | 1:1A:3715:U:O2    | 2.13                     | 0.48              |
| 1:1A:4082:G:H2'    | 1:1A:4083:U:O2    | 2.13                     | 0.48              |
| 3:1C:69:U:H2'      | 3:1C:70:G:O4'     | 2.13                     | 0.48              |
| 3:1C:99:U:OP1      | 26:2R:67:ARG:NH2  | 2.46                     | 0.48              |
| 6:1F:56:GLU:OE1    | 6:1F:56:GLU:N     | 2.40                     | 0.48              |
| 7:1G:293:ARG:HA    | 7:1G:293:ARG:HE   | 1.78                     | 0.48              |
| 10:2B:26:LYS:HG3   | 10:2B:27:VAL:H    | 1.79                     | 0.48              |
| 11:2C:60:TRP:O     | 11:2C:61:TRP:HB2  | 2.13                     | 0.48              |
| 14:2F:140:SER:O    | 14:2F:144:LEU:HG  | 2.12                     | 0.48              |
| 18:2J:2:VAL:HG13   | 18:2J:3:ARG:N     | 2.28                     | 0.48              |
| 20:2L:154:LEU:O    | 20:2L:158:GLN:HG3 | 2.13                     | 0.48              |
| 25:2Q:42:SER:O     | 25:2Q:43:LYS:HB2  | 2.12                     | 0.48              |
| 25:2Q:116:LYS:HG2  | 25:2Q:119:LYS:NZ  | 2.28                     | 0.48              |
| 32:2X:64:ILE:HG23  | 32:2X:68:LEU:HD23 | 1.95                     | 0.48              |
| 36:2b:46:LYS:N     | 36:2b:46:LYS:HD2  | 2.28                     | 0.48              |
| 44:2j:38:THR:OG1   | 44:2j:45:THR:HG22 | 2.13                     | 0.48              |
| 47:2m:189:U:OP2    | 54:2t:148:LYS:NZ  | 2.46                     | 0.48              |
| 47:2m:606:G:O2'    | 47:2m:607:U:H5''  | 2.12                     | 0.48              |
| 47:2m:892:U:HO2'   | 47:2m:893:U:P     | 2.36                     | 0.48              |
| 47:2m:980:A:O2'    | 47:2m:981:A:H5'   | 2.13                     | 0.48              |
| 47:2m:1544:C:N4    | 47:2m:1588:A:O2'  | 2.46                     | 0.48              |
| 47:2m:1545:A:O3'   | 58:2x:74:GLY:HA2  | 2.13                     | 0.48              |
| 47:2m:1674:G:OP1   | 52:2r:51:HIS:NE2  | 2.45                     | 0.48              |
| 47:2m:1818:A:C2'   | 47:2m:1819:A:H5'' | 2.43                     | 0.48              |
| 48:2n:6:ASP:HA     | 48:2n:9:GLN:HG2   | 1.94                     | 0.48              |
| 48:2n:60:LEU:CD1   | 63:3A:79:VAL:HG22 | 2.41                     | 0.48              |
| 49:2o:179:ASN:HB3  | 49:2o:183:GLU:CG  | 2.43                     | 0.48              |
| 50:2p:69:LEU:HD22  | 50:2p:86:LEU:HD13 | 1.94                     | 0.48              |
| 51:2q:71:LYS:HZ3   | 51:2q:74:GLY:HA2  | 1.78                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:2q:175:PHE:CZ   | 51:2q:222:LEU:HD11 | 2.47                     | 0.48              |
| 52:2r:139:VAL:HG23 | 66:3D:45:ASN:O     | 2.13                     | 0.48              |
| 53:2s:23:ILE:HD13  | 53:2s:50:GLU:OE2   | 2.13                     | 0.48              |
| 53:2s:171:GLU:CD   | 53:2s:171:GLU:H    | 2.21                     | 0.48              |
| 55:2u:49:MET:HB3   | 55:2u:69:TRP:CZ2   | 2.48                     | 0.48              |
| 57:2w:98:ASN:CB    | 57:2w:122:THR:HG22 | 2.42                     | 0.48              |
| 66:3D:63:ARG:NH1   | 66:3D:63:ARG:HG2   | 2.29                     | 0.48              |
| 68:3F:54:ILE:HG13  | 68:3F:55:PRO:HD2   | 1.95                     | 0.48              |
| 68:3F:116:ASP:H    | 68:3F:118:ARG:NH1  | 2.10                     | 0.48              |
| 71:3I:119:LEU:HD13 | 71:3I:159:PHE:CE1  | 2.48                     | 0.48              |
| 72:3J:49:LEU:HD12  | 72:3J:111:VAL:CG2  | 2.44                     | 0.48              |
| 1:1A:287:U:H2'     | 1:1A:288:G:H8      | 1.78                     | 0.48              |
| 1:1A:347:A:H2'     | 1:1A:348:G:H8      | 1.77                     | 0.48              |
| 1:1A:651:C:O2'     | 1:1A:652:G:H5'     | 2.14                     | 0.48              |
| 1:1A:1244:G:H2'    | 1:1A:1245:C:H6     | 1.77                     | 0.48              |
| 1:1A:1555:G:O6     | 44:2j:4:ARG:NH1    | 2.38                     | 0.48              |
| 1:1A:1566:C:H2'    | 1:1A:1567:U:H6     | 1.76                     | 0.48              |
| 1:1A:1629:G:H1     | 4:1D:208:GLU:HG2   | 1.78                     | 0.48              |
| 1:1A:1684:A:OP1    | 29:2U:47:LYS:NZ    | 2.44                     | 0.48              |
| 1:1A:2068:C:O2'    | 1:1A:2069:A:H5'    | 2.14                     | 0.48              |
| 1:1A:2299:G:OP1    | 6:1F:182:LYS:NZ    | 2.43                     | 0.48              |
| 1:1A:2668:G:H2'    | 1:1A:2669:C:H5'    | 1.94                     | 0.48              |
| 1:1A:4199:C:H2'    | 1:1A:4200:G:H5'    | 1.93                     | 0.48              |
| 1:1A:4425:G:C6     | 1:1A:4426:C:C5     | 3.01                     | 0.48              |
| 3:1C:56:G:H2'      | 3:1C:57:C:O4'      | 2.13                     | 0.48              |
| 3:1C:70:G:H5''     | 27:2S:27:ARG:CZ    | 2.42                     | 0.48              |
| 13:2E:57:VAL:O     | 13:2E:58:ARG:HB3   | 2.14                     | 0.48              |
| 14:2F:79:GLU:H     | 14:2F:79:GLU:CD    | 2.21                     | 0.48              |
| 25:2Q:73:ARG:HH22  | 70:3H:114:VAL:HG21 | 1.78                     | 0.48              |
| 36:2b:32:ARG:HG2   | 36:2b:32:ARG:NH1   | 2.27                     | 0.48              |
| 46:2l:54:ARG:CA    | 46:2l:154:THR:HG21 | 2.37                     | 0.48              |
| 46:2l:147:LYS:HZ2  | 46:2l:150:GLU:H    | 1.61                     | 0.48              |
| 47:2m:224:A:H2     | 47:2m:298:G:N1     | 2.11                     | 0.48              |
| 47:2m:1041:G:N2    | 47:2m:1042:A:N7    | 2.62                     | 0.48              |
| 47:2m:1667:U:H2'   | 47:2m:1668:U:H6    | 1.75                     | 0.48              |
| 47:2m:1679:A:C8    | 52:2r:60:ARG:HG3   | 2.48                     | 0.48              |
| 47:2m:1780:G:H2'   | 47:2m:1781:A:O5'   | 2.13                     | 0.48              |
| 48:2n:37:TYR:CG    | 48:2n:162:PRO:HG3  | 2.48                     | 0.48              |
| 48:2n:53:ARG:HD2   | 63:3A:83:PHE:CD2   | 2.48                     | 0.48              |
| 54:2t:130:THR:HA   | 54:2t:134:GLU:HB3  | 1.94                     | 0.48              |
| 55:2u:52:LEU:CD2   | 55:2u:57:TYR:HB2   | 2.44                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:3A:80:SER:C    | 63:3A:82:ASN:H     | 2.20                     | 0.48              |
| 68:3F:285:GLN:C   | 68:3F:303:THR:HG23 | 2.37                     | 0.48              |
| 69:3G:110:MET:HG3 | 69:3G:110:MET:O    | 2.11                     | 0.48              |
| 70:3H:76:LEU:HD12 | 70:3H:93:LYS:C     | 2.38                     | 0.48              |
| 70:3H:125:THR:O   | 70:3H:125:THR:OG1  | 2.31                     | 0.48              |
| 76:3N:103:SER:OG  | 76:3N:106:GLN:HG3  | 2.13                     | 0.48              |
| 77:3O:94:LYS:HB2  | 77:3O:96:LEU:CD2   | 2.43                     | 0.48              |
| 1:1A:53:C:O3'     | 1:1A:2462:C:H1'    | 2.14                     | 0.48              |
| 1:1A:60:G:H2'     | 1:1A:61:A:C8       | 2.49                     | 0.48              |
| 1:1A:137:G:C2'    | 1:1A:138:G:O4'     | 2.62                     | 0.48              |
| 1:1A:500:G:C1'    | 1:1A:504:G:H3'     | 2.44                     | 0.48              |
| 1:1A:659:G:O2'    | 1:1A:660:A:H5'     | 2.12                     | 0.48              |
| 1:1A:1092:G:H2'   | 1:1A:1093:C:C6     | 2.47                     | 0.48              |
| 1:1A:1412:G:H2'   | 1:1A:1413:C:C6     | 2.48                     | 0.48              |
| 1:1A:1412:G:O2'   | 1:1A:1413:C:H5'    | 2.14                     | 0.48              |
| 1:1A:1548:G:O2'   | 1:1A:2812:A:N3     | 2.44                     | 0.48              |
| 1:1A:2033:A:H1'   | 1:1A:2034:G:OP1    | 2.13                     | 0.48              |
| 1:1A:2348:G:H5'   | 1:1A:2351:C:C5     | 2.49                     | 0.48              |
| 1:1A:2706:G:H2'   | 1:1A:2707:U:H5''   | 1.94                     | 0.48              |
| 1:1A:3600:G:H2'   | 1:1A:3601:C:C6     | 2.48                     | 0.48              |
| 1:1A:3635:A:H2'   | 1:1A:3636:C:H5'    | 1.94                     | 0.48              |
| 1:1A:3793:U:H2'   | 1:1A:3794:C:H6     | 1.79                     | 0.48              |
| 1:1A:4593:C:O2'   | 1:1A:4594:U:H5'    | 2.12                     | 0.48              |
| 9:2A:46:ARG:O     | 9:2A:50:ILE:HG23   | 2.13                     | 0.48              |
| 13:2E:52:LYS:HA   | 13:2E:66:GLU:O     | 2.13                     | 0.48              |
| 20:2L:99:MET:HE2  | 20:2L:99:MET:CA    | 2.41                     | 0.48              |
| 20:2L:174:GLU:HG3 | 20:2L:175:GLU:N    | 2.28                     | 0.48              |
| 23:2O:38:ASN:HA   | 23:2O:41:GLN:HE21  | 1.78                     | 0.48              |
| 32:2X:90:ARG:CD   | 32:2X:102:LEU:HD23 | 2.43                     | 0.48              |
| 46:2l:172:VAL:CG1 | 46:2l:179:LEU:HD11 | 2.42                     | 0.48              |
| 46:2l:212:LYS:HD3 | 46:2l:212:LYS:H    | 1.79                     | 0.48              |
| 47:2m:297:A:H2'   | 47:2m:298:G:H5'    | 1.95                     | 0.48              |
| 47:2m:333:G:C3'   | 47:2m:334:C:H5''   | 2.43                     | 0.48              |
| 47:2m:655:A:H1'   | 47:2m:658:U:OP1    | 2.13                     | 0.48              |
| 47:2m:661:U:OP2   | 47:2m:662:G:O2'    | 2.25                     | 0.48              |
| 47:2m:1331:C:O2'  | 47:2m:1332:A:H5'   | 2.14                     | 0.48              |
| 47:2m:1440:C:C2'  | 47:2m:1441:U:H5'   | 2.43                     | 0.48              |
| 47:2m:1516:G:C2'  | 47:2m:1517:G:O5'   | 2.61                     | 0.48              |
| 47:2m:1761:U:H2'  | 47:2m:1772:C:H41   | 1.78                     | 0.48              |
| 48:2n:23:THR:HG21 | 48:2n:174:MET:SD   | 2.53                     | 0.48              |
| 48:2n:128:ARG:HA  | 48:2n:131:HIS:NE2  | 2.27                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:2o:83:LYS:HE2   | 49:2o:83:LYS:HB2   | 1.73                     | 0.48              |
| 50:2p:39:VAL:HG22  | 50:2p:48:ILE:CG1   | 2.33                     | 0.48              |
| 52:2r:126:THR:O    | 52:2r:127:ARG:HG2  | 2.13                     | 0.48              |
| 56:2v:114:SER:HB3  | 56:2v:116:CYS:SG   | 2.54                     | 0.48              |
| 57:2w:80:LEU:O     | 57:2w:80:LEU:HG    | 2.14                     | 0.48              |
| 59:2y:58:MET:HA    | 59:2y:61:ILE:HG12  | 1.95                     | 0.48              |
| 60:2z:63:GLU:HG2   | 60:2z:66:ARG:HH21  | 1.78                     | 0.48              |
| 61:20:28:LEU:HD21  | 61:20:54:TYR:CD2   | 2.49                     | 0.48              |
| 62:21:24:LEU:HD13  | 62:21:32:LEU:HD13  | 1.94                     | 0.48              |
| 64:3B:32:LEU:HD11  | 64:3B:34:THR:CG2   | 2.44                     | 0.48              |
| 68:3F:211:GLY:O    | 68:3F:236:ILE:HG22 | 2.13                     | 0.48              |
| 73:3K:93:LYS:CA    | 73:3K:150:VAL:HG21 | 2.44                     | 0.48              |
| 1:1A:99:A:H5''     | 16:2H:184:ILE:HD13 | 1.95                     | 0.48              |
| 1:1A:1667:G:H5'    | 1:1A:1688:G:OP1    | 2.13                     | 0.48              |
| 1:1A:1699:A:H4'    | 6:1F:306:ARG:NH1   | 2.28                     | 0.48              |
| 1:1A:1908:A:C2'    | 1:1A:1909:G:H5'    | 2.44                     | 0.48              |
| 1:1A:2080:U:H2'    | 1:1A:2081:C:H6     | 1.78                     | 0.48              |
| 1:1A:2358:G:C2'    | 1:1A:2359:U:H5'    | 2.43                     | 0.48              |
| 1:1A:2483:G:H2'    | 1:1A:2484:A:N9     | 2.28                     | 0.48              |
| 1:1A:2604:C:O2'    | 1:1A:2605:G:H5'    | 2.14                     | 0.48              |
| 1:1A:2652:G:C5     | 35:2a:50:PRO:HG3   | 2.49                     | 0.48              |
| 1:1A:2727:C:H2'    | 1:1A:2728:U:H6     | 1.77                     | 0.48              |
| 1:1A:3628:G:O2'    | 1:1A:3629:A:H5'    | 2.13                     | 0.48              |
| 1:1A:4119:C:H5     | 35:2a:100:GLN:HE21 | 1.61                     | 0.48              |
| 1:1A:4327:C:O2'    | 1:1A:4328:G:H5'    | 2.14                     | 0.48              |
| 1:1A:4356:G:O2'    | 1:1A:4357:G:H5'    | 2.14                     | 0.48              |
| 1:1A:4689:U:C2'    | 1:1A:4690:G:H5'    | 2.43                     | 0.48              |
| 3:1C:121:G:H2'     | 3:1C:122:G:O4'     | 2.13                     | 0.48              |
| 5:1E:163:ILE:CG2   | 5:1E:180:LEU:HD22  | 2.43                     | 0.48              |
| 5:1E:397:ILE:HG13  | 5:1E:398:ALA:N     | 2.28                     | 0.48              |
| 10:2B:167:VAL:HG12 | 10:2B:170:LEU:HD12 | 1.94                     | 0.48              |
| 33:2Y:43:ASN:O     | 33:2Y:47:ARG:HG3   | 2.13                     | 0.48              |
| 40:2f:23:ILE:HG23  | 40:2f:38:ASN:HB2   | 1.95                     | 0.48              |
| 46:2l:56:LYS:HG2   | 46:2l:152:LYS:NZ   | 2.28                     | 0.48              |
| 47:2m:42:A:H4'     | 47:2m:98:C:OP1     | 2.14                     | 0.48              |
| 47:2m:351:G:C2     | 47:2m:352:U:C6     | 3.02                     | 0.48              |
| 47:2m:1083:A:H4'   | 47:2m:1085:C:C5    | 2.48                     | 0.48              |
| 47:2m:1229:G:H2'   | 47:2m:1230:C:O4'   | 2.14                     | 0.48              |
| 47:2m:1429:G:O2'   | 61:20:7:LYS:HG3    | 2.13                     | 0.48              |
| 50:2p:21:LEU:HD12  | 50:2p:22:ASN:N     | 2.28                     | 0.48              |
| 50:2p:53:THR:O     | 50:2p:90:LYS:HD3   | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:2s:58:LYS:HE3   | 53:2s:90:LYS:HD2   | 1.96                     | 0.48              |
| 53:2s:95:ILE:HG22  | 53:2s:96:ALA:N     | 2.28                     | 0.48              |
| 61:20:110:LEU:HB3  | 61:20:112:MET:HE3  | 1.94                     | 0.48              |
| 62:21:81:GLN:CD    | 67:3E:55:LEU:HD13  | 2.38                     | 0.48              |
| 66:3D:14:VAL:CG1   | 66:3D:52:GLU:HA    | 2.43                     | 0.48              |
| 66:3D:63:ARG:HG2   | 66:3D:63:ARG:HH11  | 1.77                     | 0.48              |
| 70:3H:85:ARG:HG2   | 70:3H:87:ARG:NH1   | 2.29                     | 0.48              |
| 71:3I:28:GLU:CG    | 71:3I:40:LYS:HD3   | 2.43                     | 0.48              |
| 1:1A:225:G:OP2     | 6:1F:223:ASN:HB2   | 2.14                     | 0.48              |
| 1:1A:259:C:O2'     | 1:1A:260:C:H5'     | 2.13                     | 0.48              |
| 1:1A:437:G:O2'     | 1:1A:438:G:H5'     | 2.13                     | 0.48              |
| 1:1A:1341:U:H2'    | 1:1A:1342:A:C8     | 2.48                     | 0.48              |
| 1:1A:2638:G:O2'    | 1:1A:2639:U:H5'    | 2.14                     | 0.48              |
| 1:1A:2766:A:H2'    | 1:1A:2767:U:O4'    | 2.13                     | 0.48              |
| 1:1A:2859:G:H21    | 1:1A:3837:C:H1'    | 1.77                     | 0.48              |
| 1:1A:4130:C:H2'    | 1:1A:4131:G:C8     | 2.48                     | 0.48              |
| 1:1A:4468:U:O2     | 1:1A:4468:U:H2'    | 2.13                     | 0.48              |
| 1:1A:4731:G:H1'    | 1:1A:4732:G:P      | 2.54                     | 0.48              |
| 81:1A:5110:84D:N2  | 81:1A:5110:84D:O7  | 2.47                     | 0.48              |
| 5:1E:378:ARG:HG2   | 25:2Q:32:LEU:HD21  | 1.96                     | 0.48              |
| 6:1F:336:ARG:HG2   | 8:1H:54:ILE:CD1    | 2.44                     | 0.48              |
| 13:2E:24:ILE:HG12  | 13:2E:128:LEU:HB3  | 1.95                     | 0.48              |
| 21:2M:6:THR:HG23   | 21:2M:6:THR:O      | 2.12                     | 0.48              |
| 44:2j:28:LYS:HD3   | 44:2j:28:LYS:C     | 2.38                     | 0.48              |
| 47:2m:306:C:H2'    | 47:2m:307:G:C6     | 2.47                     | 0.48              |
| 47:2m:816:A:O2'    | 47:2m:817:G:H5'    | 2.14                     | 0.48              |
| 47:2m:841:G:P      | 76:3N:14:THR:HG22  | 2.54                     | 0.48              |
| 47:2m:1656:G:O6    | 47:2m:1669:G:C6    | 2.66                     | 0.48              |
| 48:2n:86:ALA:HB2   | 48:2n:202:TYR:O    | 2.13                     | 0.48              |
| 52:2r:16:ASP:N     | 52:2r:16:ASP:OD1   | 2.46                     | 0.48              |
| 53:2s:51:ILE:HD12  | 53:2s:52:GLU:C     | 2.38                     | 0.48              |
| 54:2t:123:ARG:NH2  | 54:2t:133:GLU:HG2  | 2.28                     | 0.48              |
| 55:2u:32:HIS:NE2   | 55:2u:42:ASN:HA    | 2.29                     | 0.48              |
| 56:2v:128:VAL:HG12 | 56:2v:142:VAL:HG22 | 1.95                     | 0.48              |
| 57:2w:90:VAL:HA    | 57:2w:107:ILE:HG21 | 1.95                     | 0.48              |
| 60:2z:109:GLU:HA   | 60:2z:112:GLU:HG2  | 1.96                     | 0.48              |
| 62:21:80:PHE:HE1   | 67:3E:54:LYS:HZ3   | 1.60                     | 0.48              |
| 68:3F:152:SER:CB   | 68:3F:169:GLY:HA2  | 2.44                     | 0.48              |
| 68:3F:199:THR:HG21 | 68:3F:240:CYS:HA   | 1.94                     | 0.48              |
| 73:3K:80:LEU:HD23  | 73:3K:80:LEU:H     | 1.79                     | 0.48              |
| 78:3P:56:CYS:HB3   | 78:3P:59:CYS:O     | 2.12                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:3R:113:LYS:NZ  | 80:3R:115:SER:HB3  | 2.28                     | 0.48              |
| 1:1A:374:G:C2'    | 1:1A:375:G:H5'     | 2.43                     | 0.48              |
| 1:1A:1180:C:H4'   | 1:1A:1180:C:OP1    | 2.14                     | 0.48              |
| 1:1A:1244:G:H2'   | 1:1A:1245:C:C6     | 2.48                     | 0.48              |
| 1:1A:1952:G:O2'   | 1:1A:1953:U:H5'    | 2.13                     | 0.48              |
| 1:1A:2677:G:H2'   | 1:1A:2678:A:H5'    | 1.95                     | 0.48              |
| 1:1A:2728:U:H2'   | 1:1A:2729:C:C6     | 2.48                     | 0.48              |
| 1:1A:3796:U:O2'   | 1:1A:3797:C:H5'    | 2.13                     | 0.48              |
| 1:1A:4057:C:H3'   | 1:1A:4057:C:H6     | 1.77                     | 0.48              |
| 1:1A:4964:C:C2'   | 1:1A:4965:U:H5'    | 2.43                     | 0.48              |
| 3:1C:79:G:H2'     | 3:1C:80:A:O4'      | 2.14                     | 0.48              |
| 4:1D:225:ILE:HG12 | 4:1D:234:LYS:HA    | 1.95                     | 0.48              |
| 6:1F:66:SER:HA    | 6:1F:77:PRO:HA     | 1.95                     | 0.48              |
| 8:1H:221:LYS:HA   | 8:1H:237:LYS:HZ1   | 1.78                     | 0.48              |
| 10:2B:125:LYS:HE3 | 10:2B:125:LYS:HB2  | 1.76                     | 0.48              |
| 11:2C:92:MET:HB3  | 11:2C:181:VAL:HA   | 1.96                     | 0.48              |
| 47:2m:550:C:OP2   | 47:2m:550:C:H3'    | 2.14                     | 0.48              |
| 47:2m:870:A:H2'   | 47:2m:870:A:P      | 2.53                     | 0.48              |
| 47:2m:884:C:C2'   | 47:2m:885:U:H5'    | 2.44                     | 0.48              |
| 47:2m:905:C:H2'   | 47:2m:906:U:C6     | 2.48                     | 0.48              |
| 47:2m:1309:C:H42  | 80:3R:100:LEU:HD21 | 1.78                     | 0.48              |
| 47:2m:1409:A:H5'  | 58:2x:24:HIS:CE1   | 2.49                     | 0.48              |
| 47:2m:1560:U:H2'  | 47:2m:1561:A:C8    | 2.49                     | 0.48              |
| 47:2m:1589:A:H4'  | 61:20:82:ARG:HG2   | 1.95                     | 0.48              |
| 47:2m:1680:G:H2'  | 47:2m:1681:U:C6    | 2.49                     | 0.48              |
| 48:2n:82:THR:O    | 48:2n:82:THR:HG22  | 2.13                     | 0.48              |
| 48:2n:222:VAL:O   | 48:2n:223:THR:OG1  | 2.25                     | 0.48              |
| 51:2q:116:PRO:O   | 51:2q:120:LYS:HG2  | 2.14                     | 0.48              |
| 53:2s:103:LYS:HB2 | 53:2s:116:ARG:NH2  | 2.29                     | 0.48              |
| 55:2u:16:PHE:CE1  | 55:2u:80:ARG:HG3   | 2.49                     | 0.48              |
| 55:2u:57:TYR:HB3  | 55:2u:75:GLY:CA    | 2.43                     | 0.48              |
| 70:3H:140:ARG:O   | 70:3H:143:LYS:HG2  | 2.13                     | 0.48              |
| 76:3N:27:VAL:HB   | 76:3N:69:THR:HG22  | 1.93                     | 0.48              |
| 1:1A:308:G:H1'    | 37:2c:31:GLY:O     | 2.14                     | 0.48              |
| 1:1A:687:U:N3     | 8:1H:95:PRO:HG2    | 2.29                     | 0.48              |
| 1:1A:704:C:O2     | 1:1A:704:C:H3'     | 2.13                     | 0.48              |
| 1:1A:1767:A:N6    | 57:2w:10:ARG:HB3   | 2.29                     | 0.48              |
| 1:1A:1926:C:O2'   | 1:1A:1927:U:H5'    | 2.13                     | 0.48              |
| 1:1A:2775:C:O2'   | 1:1A:2776:G:P      | 2.72                     | 0.48              |
| 1:1A:3596:A:OP1   | 1:1A:3596:A:H3'    | 2.13                     | 0.48              |
| 1:1A:3651:A:H2'   | 1:1A:3652:A:H8     | 1.77                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:3699:C:O2'   | 1:1A:3700:C:H5'    | 2.14                     | 0.48              |
| 1:1A:4089:G:H2'   | 1:1A:4090:G:H8     | 1.78                     | 0.48              |
| 1:1A:4212:A:H4'   | 1:1A:4213:A:N3     | 2.28                     | 0.48              |
| 1:1A:4226:G:C2'   | 1:1A:4227:U:H5'    | 2.43                     | 0.48              |
| 1:1A:4727:A:OP1   | 5:1E:132:LYS:HB2   | 2.14                     | 0.48              |
| 1:1A:4774:C:H5''  | 1:1A:4775:C:P      | 2.53                     | 0.48              |
| 1:1A:5038:A:H2'   | 1:1A:5039:U:C6     | 2.49                     | 0.48              |
| 3:1C:84:A:H4'     | 3:1C:85:U:C4'      | 2.44                     | 0.48              |
| 6:1F:65:GLU:O     | 6:1F:77:PRO:HA     | 2.13                     | 0.48              |
| 8:1H:95:PRO:HA    | 8:1H:104:THR:HG22  | 1.96                     | 0.48              |
| 8:1H:276:ALA:CB   | 34:2Z:3:GLY:HA3    | 2.44                     | 0.48              |
| 47:2m:976:G:H2'   | 47:2m:977:C:H6     | 1.79                     | 0.48              |
| 47:2m:1159:G:OP1  | 75:3M:76:SER:HB2   | 2.14                     | 0.48              |
| 47:2m:1404:U:C5   | 62:21:88:LEU:HD21  | 2.48                     | 0.48              |
| 47:2m:1421:A:O2'  | 61:20:3:GLY:N      | 2.46                     | 0.48              |
| 47:2m:1503:C:H2'  | 47:2m:1504:U:H6    | 1.75                     | 0.48              |
| 47:2m:1644:C:H4'  | 58:2x:140:ARG:HB2  | 1.95                     | 0.48              |
| 47:2m:1672:U:P    | 58:2x:18:THR:HG1   | 2.37                     | 0.48              |
| 47:2m:1702:G:H2'  | 47:2m:1703:C:O4'   | 2.14                     | 0.48              |
| 49:2o:38:MET:CE   | 49:2o:185:VAL:HG11 | 2.43                     | 0.48              |
| 50:2p:53:THR:HG22 | 50:2p:91:VAL:HG22  | 1.95                     | 0.48              |
| 55:2u:7:ASN:OD1   | 55:2u:40:VAL:HG22  | 2.13                     | 0.48              |
| 55:2u:21:MET:SD   | 55:2u:21:MET:C     | 2.96                     | 0.48              |
| 56:2v:144:LYS:HG2 | 56:2v:145:VAL:N    | 2.29                     | 0.48              |
| 57:2w:120:SER:O   | 57:2w:120:SER:OG   | 2.29                     | 0.48              |
| 60:2z:61:GLU:OE1  | 60:2z:61:GLU:HA    | 2.13                     | 0.48              |
| 67:3E:24:CYS:SG   | 67:3E:26:ASN:HB2   | 2.54                     | 0.48              |
| 68:3F:114:SER:O   | 68:3F:117:ASN:ND2  | 2.47                     | 0.48              |
| 69:3G:240:THR:O   | 69:3G:244:ILE:HG23 | 2.14                     | 0.48              |
| 70:3H:221:LYS:HE3 | 70:3H:225:GLN:OE1  | 2.13                     | 0.48              |
| 71:3I:124:HIS:HD2 | 79:3Q:31:ARG:HE    | 1.62                     | 0.48              |
| 72:3J:58:GLU:HG2  | 72:3J:58:GLU:O     | 2.13                     | 0.48              |
| 75:3M:18:GLU:HG2  | 75:3M:69:LEU:O     | 2.13                     | 0.48              |
| 1:1A:106:A:H2'    | 1:1A:107:G:O4'     | 2.13                     | 0.48              |
| 1:1A:279:A:H5'    | 1:1A:329:A:C2      | 2.49                     | 0.48              |
| 1:1A:1079:C:H2'   | 1:1A:1080:C:O4'    | 2.14                     | 0.48              |
| 1:1A:1538:U:H2'   | 1:1A:1539:G:H8     | 1.79                     | 0.48              |
| 1:1A:1732:C:C2'   | 1:1A:1733:G:H5'    | 2.43                     | 0.48              |
| 1:1A:1811:G:H2'   | 1:1A:1812:C:C6     | 2.48                     | 0.48              |
| 1:1A:2078:C:H2'   | 1:1A:2079:G:C8     | 2.49                     | 0.48              |
| 1:1A:2399:G:N2    | 35:2a:4:ARG:HD2    | 2.29                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2683:C:H2'    | 1:1A:2684:C:C6     | 2.49                     | 0.48              |
| 1:1A:3772:U:H2'    | 1:1A:3775:A:C2     | 2.45                     | 0.48              |
| 1:1A:4208:U:OP1    | 1:1A:4334:U:O2'    | 2.28                     | 0.48              |
| 1:1A:4305:G:O6     | 22:2N:80:VAL:HG11  | 2.14                     | 0.48              |
| 1:1A:4486:C:H2'    | 1:1A:4487:A:H5'    | 1.96                     | 0.48              |
| 1:1A:4705:A:H2'    | 1:1A:4706:G:O4'    | 2.14                     | 0.48              |
| 8:1H:276:ALA:HB2   | 34:2Z:3:GLY:HA3    | 1.95                     | 0.48              |
| 20:2L:47:ASP:OD1   | 20:2L:47:ASP:C     | 2.56                     | 0.48              |
| 26:2R:80:PRO:CG    | 26:2R:155:ILE:HG21 | 2.39                     | 0.48              |
| 43:2i:14:LYS:HD2   | 43:2i:77:CYS:HB3   | 1.96                     | 0.48              |
| 46:2l:206:ILE:HG23 | 46:2l:206:ILE:O    | 2.13                     | 0.48              |
| 47:2m:907:G:H2'    | 47:2m:908:A:N7     | 2.28                     | 0.48              |
| 47:2m:1433:C:H3'   | 47:2m:1434:C:C5    | 2.48                     | 0.48              |
| 49:2o:49:VAL:HG13  | 49:2o:58:ALA:HB1   | 1.96                     | 0.48              |
| 56:2v:82:MET:CG    | 56:2v:85:THR:HB    | 2.25                     | 0.48              |
| 60:2z:30:ILE:HG12  | 60:2z:71:MET:CE    | 2.40                     | 0.48              |
| 68:3F:212:LYS:O    | 68:3F:235:ILE:HG13 | 2.13                     | 0.48              |
| 68:3F:212:LYS:HG3  | 68:3F:235:ILE:CG1  | 2.43                     | 0.48              |
| 70:3H:140:ARG:HA   | 70:3H:143:LYS:CD   | 2.43                     | 0.48              |
| 78:3P:35:VAL:HG11  | 78:3P:46:VAL:CG2   | 2.44                     | 0.48              |
| 1:1A:152:U:OP2     | 16:2H:49:ARG:NH2   | 2.41                     | 0.48              |
| 1:1A:223:G:H4'     | 1:1A:225:G:N7      | 2.29                     | 0.48              |
| 1:1A:967:C:O2'     | 1:1A:968:C:H5''    | 2.14                     | 0.48              |
| 1:1A:1342:A:C2'    | 1:1A:1343:A:H5'    | 2.44                     | 0.48              |
| 1:1A:1633:G:H4'    | 1:1A:1634:A:O5'    | 2.13                     | 0.48              |
| 1:1A:2306:G:H1'    | 1:1A:2332:A:H61    | 1.79                     | 0.48              |
| 1:1A:2781:G:C2'    | 1:1A:2782:U:H5'    | 2.44                     | 0.48              |
| 1:1A:3802:U:O2'    | 1:1A:3803:A:H5'    | 2.12                     | 0.48              |
| 1:1A:3971:G:C2'    | 1:1A:3972:A:H5''   | 2.43                     | 0.48              |
| 1:1A:4642:U:H2'    | 1:1A:4643:G:H8     | 1.78                     | 0.48              |
| 2:1B:29:C:H2'      | 2:1B:29:C:O2       | 2.14                     | 0.48              |
| 2:1B:42:A:H1'      | 13:2E:75:ARG:NH1   | 2.29                     | 0.48              |
| 3:1C:131:G:O2'     | 3:1C:132:G:H5'     | 2.14                     | 0.48              |
| 12:2D:19:LYS:HB3   | 12:2D:26:VAL:HG11  | 1.96                     | 0.48              |
| 14:2F:100:PRO:O    | 37:2c:25:ARG:NH2   | 2.46                     | 0.48              |
| 14:2F:145:LYS:HG3  | 14:2F:146:LEU:HD12 | 1.96                     | 0.48              |
| 25:2Q:25:ASP:OD1   | 25:2Q:27:LYS:HG3   | 2.14                     | 0.48              |
| 27:2S:50:ARG:HG3   | 27:2S:51:LYS:N     | 2.29                     | 0.48              |
| 32:2X:33:ILE:O     | 32:2X:33:ILE:CG2   | 2.62                     | 0.48              |
| 46:2l:80:VAL:HG23  | 46:2l:82:ILE:HG23  | 1.95                     | 0.48              |
| 47:2m:207:G:HO2'   | 47:2m:208:G:P      | 2.32                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:337:C:H2'   | 47:2m:338:G:C4'    | 2.33                     | 0.48              |
| 47:2m:1589:A:H4'  | 61:20:82:ARG:HG3   | 1.95                     | 0.48              |
| 51:2q:72:ILE:HD12 | 51:2q:77:ARG:CG    | 2.44                     | 0.48              |
| 53:2s:46:THR:HG21 | 53:2s:97:GLN:CG    | 2.44                     | 0.48              |
| 57:2w:81:ARG:HA   | 57:2w:116:LEU:CD1  | 2.34                     | 0.48              |
| 67:3E:8:TRP:CG    | 67:3E:8:TRP:O      | 2.67                     | 0.48              |
| 68:3F:103:GLY:HA3 | 68:3F:132:TRP:CZ2  | 2.49                     | 0.48              |
| 68:3F:177:TRP:HE1 | 68:3F:184:LEU:HD13 | 1.78                     | 0.48              |
| 77:3O:47:LEU:CB   | 77:3O:79:ILE:HA    | 2.39                     | 0.48              |
| 77:3O:63:PRO:HB2  | 77:3O:96:LEU:HD12  | 1.95                     | 0.48              |
| 1:1A:272:U:O2'    | 1:1A:273:U:H5'     | 2.14                     | 0.47              |
| 1:1A:360:A:H4'    | 1:1A:361:C:OP2     | 2.14                     | 0.47              |
| 1:1A:443:G:O2'    | 1:1A:444:G:H5'     | 2.14                     | 0.47              |
| 1:1A:649:A:O2'    | 1:1A:650:C:H5'     | 2.14                     | 0.47              |
| 1:1A:1079:C:C2'   | 1:1A:1080:C:O4'    | 2.62                     | 0.47              |
| 1:1A:1770:A:O2'   | 1:1A:1771:U:H5'    | 2.14                     | 0.47              |
| 1:1A:1772:C:H2'   | 1:1A:1773:U:C6     | 2.49                     | 0.47              |
| 1:1A:2262:G:P     | 45:2k:94:ARG:HD3   | 2.54                     | 0.47              |
| 1:1A:2504:C:HO2'  | 1:1A:2505:C:P      | 2.37                     | 0.47              |
| 1:1A:3756:A:H61   | 1:1A:3767:C:N4     | 2.12                     | 0.47              |
| 1:1A:3975:C:H2'   | 1:1A:3976:C:C5     | 2.48                     | 0.47              |
| 1:1A:4197:G:C4    | 1:1A:4198:G:C8     | 3.02                     | 0.47              |
| 1:1A:4305:G:H22   | 22:2N:87:LYS:HD3   | 1.79                     | 0.47              |
| 6:1F:193:LYS:CD   | 6:1F:196:MET:HE3   | 2.44                     | 0.47              |
| 7:1G:182:GLY:CA   | 7:1G:194:VAL:HG22  | 2.38                     | 0.47              |
| 8:1H:114:ARG:HG2  | 8:1H:114:ARG:O     | 2.13                     | 0.47              |
| 19:2K:122:THR:OG1 | 19:2K:125:GLN:HG3  | 2.14                     | 0.47              |
| 23:2O:78:PHE:CE1  | 23:2O:83:LEU:HD13  | 2.49                     | 0.47              |
| 27:2S:82:ILE:CG2  | 27:2S:83:GLU:N     | 2.77                     | 0.47              |
| 28:2T:73:LYS:HD3  | 28:2T:75:TYR:CE1   | 2.49                     | 0.47              |
| 28:2T:92:ASP:OD1  | 28:2T:94:THR:HG22  | 2.14                     | 0.47              |
| 32:2X:33:ILE:CD1  | 32:2X:44:ARG:HG3   | 2.44                     | 0.47              |
| 37:2c:70:LEU:HB2  | 37:2c:87:ARG:HH11  | 1.78                     | 0.47              |
| 43:2i:20:PRO:O    | 43:2i:73:VAL:HG22  | 2.14                     | 0.47              |
| 47:2m:7:G:O2'     | 47:2m:622:C:H4'    | 2.14                     | 0.47              |
| 47:2m:43:U:OP2    | 47:2m:485:A:N6     | 2.33                     | 0.47              |
| 47:2m:694:G:C6    | 47:2m:738:C:H4'    | 2.49                     | 0.47              |
| 47:2m:1235:G:N2   | 57:2w:135:ALA:HB2  | 2.22                     | 0.47              |
| 47:2m:1286:G:H1   | 47:2m:1312:G:HO2'  | 1.60                     | 0.47              |
| 47:2m:1512:C:O2'  | 47:2m:1513:C:H6    | 1.97                     | 0.47              |
| 50:2p:30:ALA:O    | 50:2p:103:GLU:HG2  | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:2q:60:GLU:O     | 51:2q:63:LYS:HG2   | 2.14                     | 0.47              |
| 51:2q:139:LEU:HD23 | 51:2q:147:ILE:HB   | 1.94                     | 0.47              |
| 57:2w:67:ALA:CB    | 57:2w:73:PRO:HG3   | 2.43                     | 0.47              |
| 63:3A:51:LYS:NZ    | 63:3A:76:ASP:HB3   | 2.29                     | 0.47              |
| 64:3B:82:THR:HG23  | 64:3B:118:VAL:HG22 | 1.96                     | 0.47              |
| 65:3C:51:ARG:O     | 65:3C:51:ARG:HD3   | 2.14                     | 0.47              |
| 66:3D:14:VAL:HG12  | 66:3D:53:GLY:H     | 1.79                     | 0.47              |
| 68:3F:113:PHE:CE1  | 68:3F:120:ILE:HD13 | 2.49                     | 0.47              |
| 70:3H:49:VAL:HG22  | 70:3H:115:LYS:HE3  | 1.96                     | 0.47              |
| 1:1A:227:A:H61     | 1:1A:241:G:C2'     | 2.27                     | 0.47              |
| 1:1A:248:C:C2      | 1:1A:249:C:C6      | 3.02                     | 0.47              |
| 1:1A:270:U:H2'     | 1:1A:271:C:C6      | 2.49                     | 0.47              |
| 1:1A:1341:U:O2'    | 1:1A:1342:A:H5'    | 2.14                     | 0.47              |
| 1:1A:1443:A:H2'    | 1:1A:1444:G:C8     | 2.49                     | 0.47              |
| 1:1A:1953:U:H2'    | 1:1A:1954:U:H6     | 1.78                     | 0.47              |
| 1:1A:1970:A:H5'    | 1:1A:1971:C:C1'    | 2.44                     | 0.47              |
| 1:1A:3773:U:O5'    | 1:1A:3774:A:H3'    | 2.14                     | 0.47              |
| 1:1A:3832:U:H2'    | 1:1A:3833:C:C6     | 2.49                     | 0.47              |
| 1:1A:4123:C:H2'    | 1:1A:4124:G:O4'    | 2.14                     | 0.47              |
| 3:1C:71:A:C2       | 3:1C:88:A:C1'      | 2.97                     | 0.47              |
| 7:1G:203:ASN:OD1   | 7:1G:203:ASN:N     | 2.45                     | 0.47              |
| 8:1H:190:HIS:CE1   | 8:1H:192:LYS:HB2   | 2.49                     | 0.47              |
| 10:2B:173:LEU:O    | 10:2B:177:MET:HG2  | 2.14                     | 0.47              |
| 11:2C:3:THR:O      | 11:2C:61:TRP:HA    | 2.14                     | 0.47              |
| 15:2G:130:LEU:HD23 | 17:2I:177:LEU:CD2  | 2.44                     | 0.47              |
| 34:2Z:41:PHE:HZ    | 34:2Z:105:LEU:HD13 | 1.79                     | 0.47              |
| 47:2m:509:G:H5''   | 71:3I:2:PRO:O      | 2.14                     | 0.47              |
| 47:2m:940:U:H3     | 47:2m:1002:U:H3    | 1.61                     | 0.47              |
| 47:2m:1373:C:H5'   | 59:2y:7:LYS:HG3    | 1.96                     | 0.47              |
| 47:2m:1512:C:O2'   | 47:2m:1513:C:C6    | 2.67                     | 0.47              |
| 47:2m:1521:C:N4    | 60:2z:137:LYS:HG3  | 2.29                     | 0.47              |
| 47:2m:1522:A:H4'   | 60:2z:144:ARG:HD2  | 1.96                     | 0.47              |
| 47:2m:1616:U:H3    | 47:2m:1620:A:H2    | 1.61                     | 0.47              |
| 47:2m:1806:A:O2'   | 47:2m:1807:C:H5'   | 2.14                     | 0.47              |
| 49:2o:108:ASP:OD1  | 49:2o:108:ASP:N    | 2.46                     | 0.47              |
| 49:2o:136:ARG:HG2  | 49:2o:138:PHE:CE1  | 2.49                     | 0.47              |
| 53:2s:58:LYS:HB3   | 53:2s:90:LYS:CD    | 2.44                     | 0.47              |
| 55:2u:26:ASP:OD1   | 55:2u:26:ASP:N     | 2.47                     | 0.47              |
| 56:2v:144:LYS:HE3  | 56:2v:144:LYS:HB3  | 1.60                     | 0.47              |
| 57:2w:25:LEU:HD11  | 57:2w:87:PRO:HG3   | 1.95                     | 0.47              |
| 58:2x:97:GLN:NE2   | 68:3F:58:ALA:HB3   | 2.28                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 59:2y:34:VAL:HG13 | 59:2y:37:GLU:OE2   | 2.14                     | 0.47              |
| 63:3A:46:PHE:CZ   | 63:3A:48:GLY:HA2   | 2.49                     | 0.47              |
| 68:3F:15:ASN:HA   | 68:3F:305:ASN:CG   | 2.38                     | 0.47              |
| 70:3H:195:LYS:O   | 70:3H:198:ARG:HG2  | 2.14                     | 0.47              |
| 70:3H:231:ARG:HD3 | 70:3H:232:ARG:NH1  | 2.29                     | 0.47              |
| 72:3J:48:HIS:O    | 72:3J:74:ILE:HD13  | 2.13                     | 0.47              |
| 72:3J:100:PRO:HB2 | 72:3J:103:VAL:HB   | 1.95                     | 0.47              |
| 1:1A:137:G:H2'    | 1:1A:138:G:O4'     | 2.14                     | 0.47              |
| 1:1A:189:G:N3     | 1:1A:253:G:N2      | 2.62                     | 0.47              |
| 1:1A:494:U:H1'    | 1:1A:660:A:C2      | 2.49                     | 0.47              |
| 1:1A:499:G:O2'    | 1:1A:500:G:P       | 2.71                     | 0.47              |
| 1:1A:675:C:O2'    | 1:1A:676:C:H5'     | 2.15                     | 0.47              |
| 1:1A:1351:G:H2'   | 1:1A:1352:C:C6     | 2.50                     | 0.47              |
| 1:1A:1759:G:H22   | 1:1A:1773:U:H3     | 1.63                     | 0.47              |
| 1:1A:2406:G:C2'   | 1:1A:2407:G:H5'    | 2.44                     | 0.47              |
| 1:1A:2431:A:O2'   | 1:1A:2432:U:H5'    | 2.14                     | 0.47              |
| 1:1A:2480:G:H2'   | 1:1A:2481:G:C8     | 2.49                     | 0.47              |
| 1:1A:2541:G:O2'   | 1:1A:2542:G:H5'    | 2.14                     | 0.47              |
| 1:1A:3960:A:C5    | 1:1A:3961:G:H1'    | 2.49                     | 0.47              |
| 1:1A:4089:G:H2'   | 1:1A:4090:G:C8     | 2.49                     | 0.47              |
| 1:1A:4345:C:H2'   | 1:1A:4346:U:H6     | 1.80                     | 0.47              |
| 1:1A:4508:C:N3    | 1:1A:4512:U:H5     | 2.12                     | 0.47              |
| 1:1A:4769:G:H2'   | 1:1A:4770:U:H4'    | 1.97                     | 0.47              |
| 1:1A:4870:G:H21   | 1:1A:4870:G:P      | 2.37                     | 0.47              |
| 1:1A:4997:G:O2'   | 1:1A:4998:G:H5'    | 2.14                     | 0.47              |
| 3:1C:6:C:H2'      | 3:1C:7:U:C6        | 2.49                     | 0.47              |
| 3:1C:26:C:H2'     | 3:1C:27:U:C6       | 2.49                     | 0.47              |
| 7:1G:260:GLU:CG   | 7:1G:260:GLU:O     | 2.61                     | 0.47              |
| 12:2D:34:PHE:CD2  | 12:2D:89:VAL:HG23  | 2.49                     | 0.47              |
| 13:2E:64:ARG:HG2  | 13:2E:65:ASN:OD1   | 2.14                     | 0.47              |
| 15:2G:86:TRP:C    | 15:2G:88:ALA:H     | 2.22                     | 0.47              |
| 16:2H:13:LYS:HD2  | 37:2c:48:CYS:SG    | 2.54                     | 0.47              |
| 23:2O:20:LYS:HB2  | 23:2O:20:LYS:HZ2   | 1.79                     | 0.47              |
| 28:2T:83:THR:HG22 | 35:2a:95:PHE:CZ    | 2.50                     | 0.47              |
| 31:2W:99:PRO:HG3  | 31:2W:104:ILE:HD13 | 1.96                     | 0.47              |
| 43:2i:99:ARG:HG2  | 43:2i:99:ARG:NH1   | 2.28                     | 0.47              |
| 46:2l:106:LYS:HD2 | 46:2l:107:TYR:N    | 2.30                     | 0.47              |
| 47:2m:85:A:H4'    | 47:2m:150:A:H4'    | 1.95                     | 0.47              |
| 47:2m:149:A:C2    | 47:2m:150:A:H1'    | 2.50                     | 0.47              |
| 47:2m:355:G:OP1   | 56:2v:105:ARG:NH1  | 2.33                     | 0.47              |
| 47:2m:398:A:H4'   | 47:2m:399:C:H5'    | 1.94                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:476:A:H2     | 47:2m:488:U:O2     | 1.98                     | 0.47              |
| 47:2m:647:U:O2'    | 47:2m:648:A:H5'    | 2.13                     | 0.47              |
| 47:2m:882:U:O2'    | 47:2m:883:U:C6     | 2.64                     | 0.47              |
| 47:2m:1043:G:O2'   | 47:2m:1044:G:H5'   | 2.14                     | 0.47              |
| 47:2m:1105:G:O2'   | 47:2m:1106:C:H5'   | 2.13                     | 0.47              |
| 47:2m:1109:C:O2'   | 47:2m:1110:G:P     | 2.72                     | 0.47              |
| 47:2m:1204:A:O2'   | 47:2m:1700:C:OP2   | 2.25                     | 0.47              |
| 47:2m:1240:A:N6    | 47:2m:1241:A:N1    | 2.62                     | 0.47              |
| 47:2m:1402:A:OP2   | 47:2m:1402:A:H8    | 1.97                     | 0.47              |
| 49:2o:86:LEU:HA    | 49:2o:99:ASN:O     | 2.13                     | 0.47              |
| 50:2p:98:ALA:HA    | 50:2p:188:ILE:HD11 | 1.95                     | 0.47              |
| 53:2s:19:PHE:CD1   | 53:2s:23:ILE:HD11  | 2.49                     | 0.47              |
| 54:2t:119:LEU:HD11 | 54:2t:153:LYS:HG2  | 1.95                     | 0.47              |
| 56:2v:30:LYS:CG    | 56:2v:31:GLU:H     | 2.25                     | 0.47              |
| 57:2w:34:MET:HE3   | 57:2w:45:LEU:CB    | 2.43                     | 0.47              |
| 58:2x:85:ARG:HG2   | 58:2x:119:LEU:HD21 | 1.96                     | 0.47              |
| 60:2z:6:PRO:CD     | 77:3O:49:LEU:HD13  | 2.43                     | 0.47              |
| 60:2z:15:VAL:HG12  | 60:2z:16:LEU:CD1   | 2.45                     | 0.47              |
| 62:21:32:LEU:HD12  | 62:21:32:LEU:O     | 2.15                     | 0.47              |
| 65:3C:51:ARG:O     | 65:3C:55:GLU:HG3   | 2.14                     | 0.47              |
| 68:3F:292:SER:HB3  | 68:3F:297:THR:O    | 2.14                     | 0.47              |
| 69:3G:176:LYS:HD2  | 69:3G:176:LYS:O    | 2.14                     | 0.47              |
| 73:3K:94:LYS:O     | 73:3K:98:VAL:HG23  | 2.14                     | 0.47              |
| 1:1A:43:U:H2'      | 1:1A:44:A:H5'      | 1.95                     | 0.47              |
| 1:1A:240:G:H2'     | 1:1A:241:G:O4'     | 2.14                     | 0.47              |
| 1:1A:727:C:H2'     | 1:1A:728:U:C6      | 2.49                     | 0.47              |
| 1:1A:743:G:H2'     | 1:1A:744:G:O4'     | 2.14                     | 0.47              |
| 1:1A:1563:A:H2'    | 1:1A:1564:A:H8     | 1.71                     | 0.47              |
| 1:1A:2088:A:OP2    | 19:2K:37:ARG:NH2   | 2.46                     | 0.47              |
| 1:1A:2389:A:C5'    | 32:2X:70:LYS:HD2   | 2.44                     | 0.47              |
| 1:1A:2570:U:H2'    | 1:1A:2571:C:H6     | 1.78                     | 0.47              |
| 1:1A:2605:G:O2'    | 1:1A:2606:G:H5'    | 2.14                     | 0.47              |
| 1:1A:2611:A:H5''   | 1:1A:2688:G:H4'    | 1.95                     | 0.47              |
| 1:1A:2675:G:O2'    | 1:1A:2676:A:O5'    | 2.31                     | 0.47              |
| 1:1A:2690:C:H2'    | 1:1A:2691:U:O4'    | 2.14                     | 0.47              |
| 1:1A:4526:U:HO2'   | 1:1A:4527:G:H5'    | 1.78                     | 0.47              |
| 81:1A:5105:84D:O2  | 81:1A:5105:84D:O4  | 2.32                     | 0.47              |
| 2:1B:110:G:H2'     | 2:1B:111:C:H6      | 1.79                     | 0.47              |
| 5:1E:200:ARG:HG2   | 5:1E:200:ARG:HH11  | 1.79                     | 0.47              |
| 13:2E:174:ILE:O    | 13:2E:175:LEU:HB2  | 2.14                     | 0.47              |
| 14:2F:175:ASN:C    | 14:2F:175:ASN:OD1  | 2.57                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:2H:115:VAL:HG22 | 16:2H:134:LEU:CD1  | 2.44                     | 0.47              |
| 17:2I:61:ARG:HG2   | 17:2I:66:PRO:HB3   | 1.96                     | 0.47              |
| 21:2M:107:THR:O    | 21:2M:111:ARG:HG2  | 2.14                     | 0.47              |
| 47:2m:161:U:O2'    | 70:3H:87:ARG:NH2   | 2.46                     | 0.47              |
| 47:2m:339:A:H5''   | 47:2m:340:C:C6     | 2.50                     | 0.47              |
| 47:2m:407:G:H3'    | 47:2m:408:A:C5'    | 2.44                     | 0.47              |
| 47:2m:798:A:H5'    | 47:2m:800:U:P      | 2.54                     | 0.47              |
| 47:2m:1373:C:O2'   | 47:2m:1374:C:H5'   | 2.15                     | 0.47              |
| 47:2m:1402:A:H4'   | 62:21:51:LYS:CE    | 2.44                     | 0.47              |
| 50:2p:110:LEU:HG   | 50:2p:175:VAL:HG13 | 1.95                     | 0.47              |
| 54:2t:143:LYS:HA   | 54:2t:146:GLN:HG2  | 1.96                     | 0.47              |
| 55:2u:92:ALA:O     | 55:2u:96:ARG:HG2   | 2.14                     | 0.47              |
| 57:2w:108:LYS:HG2  | 57:2w:109:PRO:HD2  | 1.96                     | 0.47              |
| 60:2z:92:ASP:CG    | 60:2z:94:LYS:HB2   | 2.39                     | 0.47              |
| 62:21:21:ARG:HB3   | 62:21:115:THR:CG2  | 2.43                     | 0.47              |
| 62:21:22:ILE:CD1   | 62:21:114:VAL:HG12 | 2.43                     | 0.47              |
| 66:3D:18:LEU:HB2   | 66:3D:29:GLN:CB    | 2.44                     | 0.47              |
| 72:3J:38:ALA:O     | 72:3J:42:LEU:HG    | 2.14                     | 0.47              |
| 75:3M:97:ARG:HB3   | 75:3M:97:ARG:CZ    | 2.44                     | 0.47              |
| 76:3N:25:ILE:CD1   | 76:3N:57:VAL:HG12  | 2.44                     | 0.47              |
| 76:3N:106:GLN:O    | 76:3N:109:GLU:HG2  | 2.15                     | 0.47              |
| 77:3O:68:ILE:HG22  | 77:3O:88:LEU:HD23  | 1.95                     | 0.47              |
| 77:3O:88:LEU:HA    | 77:3O:91:LEU:HD12  | 1.95                     | 0.47              |
| 1:1A:495:C:C1'     | 1:1A:659:G:N2      | 2.78                     | 0.47              |
| 1:1A:513:U:O2      | 1:1A:516:C:H5      | 1.96                     | 0.47              |
| 1:1A:985:C:N4      | 1:1A:1068:G:O6     | 2.19                     | 0.47              |
| 1:1A:1438:U:C3'    | 1:1A:1439:C:C5'    | 2.90                     | 0.47              |
| 1:1A:1523:A:N3     | 1:1A:4389:C:O2'    | 2.45                     | 0.47              |
| 1:1A:1870:C:H2'    | 1:1A:1871:A:H8     | 1.80                     | 0.47              |
| 1:1A:2108:G:H2'    | 1:1A:2109:G:C8     | 2.49                     | 0.47              |
| 1:1A:3653:A:C2     | 1:1A:3692:A:H4'    | 2.50                     | 0.47              |
| 1:1A:3690:U:H5'    | 1:1A:3818:U:OP2    | 2.15                     | 0.47              |
| 1:1A:3773:U:HO2'   | 1:1A:3774:A:P      | 2.33                     | 0.47              |
| 1:1A:3813:A:N3     | 1:1A:4538:G:O2'    | 2.38                     | 0.47              |
| 1:1A:4324:A:H2'    | 1:1A:4325:A:C8     | 2.49                     | 0.47              |
| 1:1A:4939:C:H5''   | 1:1A:4940:C:O5'    | 2.14                     | 0.47              |
| 1:1A:4993:G:C6     | 1:1A:5058:A:N1     | 2.82                     | 0.47              |
| 3:1C:40:A:H2'      | 3:1C:41:A:C8       | 2.49                     | 0.47              |
| 6:1F:230:LEU:HG    | 6:1F:235:LEU:HD23  | 1.95                     | 0.47              |
| 8:1H:47:ASN:HB2    | 8:1H:62:MET:CE     | 2.41                     | 0.47              |
| 10:2B:175:ARG:HD2  | 10:2B:175:ARG:O    | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:2H:68:ARG:HD3   | 16:2H:124:ASP:O    | 2.14                     | 0.47              |
| 20:2L:173:ARG:HD3  | 47:2m:910:G:P      | 2.55                     | 0.47              |
| 25:2Q:14:TYR:CB    | 25:2Q:15:PRO:HD2   | 2.40                     | 0.47              |
| 26:2R:52:LEU:HD12  | 26:2R:54:LEU:CD2   | 2.45                     | 0.47              |
| 43:2i:20:PRO:HB2   | 43:2i:73:VAL:HG21  | 1.96                     | 0.47              |
| 47:2m:383:G:O2'    | 47:2m:384:U:H5'    | 2.14                     | 0.47              |
| 47:2m:560:A:C5'    | 71:3I:174:LYS:HG3  | 2.45                     | 0.47              |
| 47:2m:659:G:H5'    | 47:2m:660:C:OP1    | 2.15                     | 0.47              |
| 47:2m:898:U:H5'    | 47:2m:899:U:OP1    | 2.14                     | 0.47              |
| 47:2m:904:A:O2'    | 47:2m:905:C:H5'    | 2.14                     | 0.47              |
| 47:2m:952:G:H2'    | 47:2m:953:C:C6     | 2.49                     | 0.47              |
| 47:2m:952:G:O2'    | 47:2m:953:C:H5'    | 2.15                     | 0.47              |
| 47:2m:1431:G:N2    | 61:20:68:GLY:HA3   | 2.29                     | 0.47              |
| 47:2m:1736:G:H2'   | 47:2m:1737:G:C8    | 2.49                     | 0.47              |
| 47:2m:1740:C:H2'   | 47:2m:1741:U:C6    | 2.50                     | 0.47              |
| 48:2n:76:VAL:HG12  | 48:2n:175:TRP:CH2  | 2.49                     | 0.47              |
| 51:2q:192:ILE:CG1  | 51:2q:243:GLY:HA3  | 2.45                     | 0.47              |
| 51:2q:246:LEU:HB2  | 51:2q:251:GLU:CD   | 2.40                     | 0.47              |
| 54:2t:139:LYS:HE3  | 54:2t:141:ARG:HD2  | 1.97                     | 0.47              |
| 54:2t:166:PHE:CZ   | 54:2t:171:LEU:HD11 | 2.50                     | 0.47              |
| 55:2u:52:LEU:HD21  | 55:2u:57:TYR:HB2   | 1.96                     | 0.47              |
| 55:2u:78:TYR:HA    | 55:2u:81:ASP:OD2   | 2.14                     | 0.47              |
| 58:2x:97:GLN:OE1   | 58:2x:102:GLU:HG2  | 2.14                     | 0.47              |
| 68:3F:23:THR:HB    | 68:3F:31:ILE:HG13  | 1.95                     | 0.47              |
| 69:3G:204:ILE:HD12 | 69:3G:215:MET:HG3  | 1.97                     | 0.47              |
| 76:3N:102:THR:HG21 | 76:3N:130:LYS:HD2  | 1.96                     | 0.47              |
| 77:3O:60:LYS:HG3   | 77:3O:61:GLU:OE1   | 2.14                     | 0.47              |
| 1:1A:248:C:C2      | 1:1A:249:C:C5      | 3.03                     | 0.47              |
| 1:1A:270:U:H2'     | 1:1A:271:C:H6      | 1.78                     | 0.47              |
| 1:1A:370:U:O2'     | 1:1A:371:A:H5'     | 2.14                     | 0.47              |
| 1:1A:2575:U:H5''   | 1:1A:2576:G:H5''   | 1.97                     | 0.47              |
| 1:1A:2767:U:H4'    | 1:1A:2768:C:OP2    | 2.15                     | 0.47              |
| 1:1A:3585:G:O6     | 1:1A:3586:G:N2     | 2.48                     | 0.47              |
| 1:1A:3773:U:H4'    | 1:1A:3774:A:H5''   | 1.97                     | 0.47              |
| 1:1A:3829:G:N3     | 1:1A:3829:G:H2'    | 2.29                     | 0.47              |
| 1:1A:4047:A:H3'    | 1:1A:4047:A:N3     | 2.30                     | 0.47              |
| 1:1A:4300:U:H2'    | 1:1A:4301:U:C6     | 2.49                     | 0.47              |
| 1:1A:4303:C:O2'    | 1:1A:4304:A:H2'    | 2.15                     | 0.47              |
| 1:1A:4325:A:H4'    | 7:1G:145:TYR:CD1   | 2.48                     | 0.47              |
| 1:1A:4349:C:H3'    | 1:1A:4350:C:C5'    | 2.44                     | 0.47              |
| 1:1A:4417:C:H2'    | 1:1A:4418:G:O4'    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:4612:C:C2'   | 1:1A:4613:C:H5'   | 2.44                     | 0.47              |
| 1:1A:4615:C:O2'   | 1:1A:4616:A:H5'   | 2.14                     | 0.47              |
| 1:1A:4652:G:H2'   | 1:1A:4653:C:C6    | 2.49                     | 0.47              |
| 1:1A:4690:G:O6    | 1:1A:4698:C:H5''  | 2.14                     | 0.47              |
| 2:1B:20:U:O2'     | 2:1B:21:G:H5'     | 2.15                     | 0.47              |
| 3:1C:18:U:H2'     | 3:1C:19:C:H6      | 1.78                     | 0.47              |
| 3:1C:38:U:H3'     | 3:1C:39:G:C5'     | 2.45                     | 0.47              |
| 7:1G:181:PRO:HD2  | 7:1G:195:HIS:CD2  | 2.50                     | 0.47              |
| 12:2D:187:LYS:O   | 12:2D:188:LYS:HB2 | 2.14                     | 0.47              |
| 16:2H:166:SER:O   | 16:2H:170:LYS:HG3 | 2.14                     | 0.47              |
| 28:2T:74:VAL:O    | 28:2T:74:VAL:HG12 | 2.15                     | 0.47              |
| 42:2h:3:ALA:HB3   | 47:2m:1842:C:OP1  | 2.15                     | 0.47              |
| 47:2m:153:G:H21   | 70:3H:13:GLN:HE22 | 1.63                     | 0.47              |
| 47:2m:363:A:O3'   | 47:2m:364:A:H4'   | 2.15                     | 0.47              |
| 47:2m:1060:A:H2'  | 47:2m:1060:A:N3   | 2.30                     | 0.47              |
| 47:2m:1227:G:H2'  | 47:2m:1227:G:N3   | 2.29                     | 0.47              |
| 47:2m:1505:U:H5'  | 47:2m:1506:A:OP1  | 2.14                     | 0.47              |
| 47:2m:1560:U:H4'  | 47:2m:1583:C:HO2' | 1.78                     | 0.47              |
| 53:2s:8:ILE:HD12  | 53:2s:9:VAL:HG13  | 1.97                     | 0.47              |
| 54:2t:46:VAL:HG13 | 54:2t:54:LYS:CG   | 2.44                     | 0.47              |
| 55:2u:24:LYS:HD2  | 55:2u:25:LYS:N    | 2.30                     | 0.47              |
| 56:2v:25:LEU:HD13 | 56:2v:25:LEU:N    | 2.28                     | 0.47              |
| 57:2w:18:ARG:NH1  | 60:2z:90:VAL:HG22 | 2.28                     | 0.47              |
| 62:21:65:THR:HG23 | 62:21:67:LYS:N    | 2.30                     | 0.47              |
| 68:3F:208:ALA:CB  | 68:3F:218:LEU:HG  | 2.41                     | 0.47              |
| 71:3I:15:THR:CG2  | 71:3I:16:PRO:HD2  | 2.45                     | 0.47              |
| 77:3O:53:ALA:O    | 77:3O:57:LYS:HG2  | 2.14                     | 0.47              |
| 1:1A:183:C:O2'    | 1:1A:184:U:O2     | 2.24                     | 0.47              |
| 1:1A:266:C:H3'    | 1:1A:266:C:P      | 2.55                     | 0.47              |
| 1:1A:383:A:O2'    | 1:1A:384:A:C8     | 2.65                     | 0.47              |
| 1:1A:492:U:H2'    | 1:1A:493:G:O4'    | 2.14                     | 0.47              |
| 1:1A:733:A:C2     | 1:1A:734:G:H1'    | 2.49                     | 0.47              |
| 1:1A:934:C:H4'    | 1:1A:936:C:OP2    | 2.14                     | 0.47              |
| 1:1A:990:C:C4     | 1:1A:992:C:H1'    | 2.49                     | 0.47              |
| 1:1A:993:G:N1     | 1:1A:1050:C:H2'   | 2.26                     | 0.47              |
| 1:1A:1422:G:O2'   | 1:1A:1423:U:H5'   | 2.15                     | 0.47              |
| 1:1A:1645:C:H2'   | 1:1A:1646:A:C8    | 2.50                     | 0.47              |
| 1:1A:1693:U:H2'   | 1:1A:1694:C:O4'   | 2.14                     | 0.47              |
| 1:1A:2017:A:H3'   | 1:1A:2018:C:C5    | 2.50                     | 0.47              |
| 1:1A:2347:A:C4    | 33:2Y:31:ILE:HD11 | 2.50                     | 0.47              |
| 1:1A:2368:A:N6    | 1:1A:2827:G:O2'   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2415:U:O2'   | 1:1A:2416:G:H5'   | 2.14                     | 0.47              |
| 1:1A:2505:C:H1'   | 1:1A:2506:G:C2    | 2.50                     | 0.47              |
| 1:1A:2545:U:H5''  | 1:1A:2546:G:C4'   | 2.44                     | 0.47              |
| 1:1A:2602:G:O4'   | 1:1A:2742:G:H2'   | 2.14                     | 0.47              |
| 1:1A:2675:G:O2'   | 1:1A:2676:A:P     | 2.73                     | 0.47              |
| 1:1A:2732:G:H2'   | 1:1A:2733:C:C6    | 2.50                     | 0.47              |
| 1:1A:3715:U:H5    | 1:1A:3738:G:O6    | 1.96                     | 0.47              |
| 1:1A:3837:C:H2'   | 1:1A:3838:U:O4'   | 2.15                     | 0.47              |
| 1:1A:4277:G:H2'   | 1:1A:4278:C:C6    | 2.50                     | 0.47              |
| 1:1A:4357:G:O2'   | 1:1A:4358:U:H5'   | 2.14                     | 0.47              |
| 1:1A:4413:C:C2'   | 1:1A:4414:A:H5'   | 2.44                     | 0.47              |
| 1:1A:4453:C:O2'   | 1:1A:4454:G:H5'   | 2.15                     | 0.47              |
| 1:1A:4468:U:O2    | 1:1A:4708:A:C8    | 2.67                     | 0.47              |
| 1:1A:4538:G:H2'   | 1:1A:4539:U:H6    | 1.78                     | 0.47              |
| 3:1C:5:U:H2'      | 3:1C:6:C:H6       | 1.79                     | 0.47              |
| 3:1C:16:G:O2'     | 3:1C:17:A:H8      | 1.96                     | 0.47              |
| 5:1E:369:ASP:OD1  | 5:1E:371:THR:OG1  | 2.27                     | 0.47              |
| 7:1G:187:SER:OG   | 7:1G:189:GLU:HB2  | 2.15                     | 0.47              |
| 8:1H:216:TYR:OH   | 8:1H:246:ARG:HD2  | 2.15                     | 0.47              |
| 8:1H:261:ILE:HD13 | 8:1H:271:LEU:CD2  | 2.44                     | 0.47              |
| 9:2A:126:ASN:HB2  | 22:2N:132:PRO:O   | 2.15                     | 0.47              |
| 13:2E:21:CYS:HB2  | 13:2E:131:TYR:O   | 2.14                     | 0.47              |
| 20:2L:95:TRP:CE2  | 20:2L:99:MET:HE3  | 2.49                     | 0.47              |
| 20:2L:99:MET:HE2  | 20:2L:99:MET:N    | 2.30                     | 0.47              |
| 23:2O:31:ASP:OD1  | 23:2O:31:ASP:O    | 2.33                     | 0.47              |
| 27:2S:91:ASN:OD1  | 27:2S:93:THR:HG23 | 2.14                     | 0.47              |
| 30:2V:65:MET:HA   | 30:2V:68:ARG:HH21 | 1.80                     | 0.47              |
| 31:2W:31:TYR:OH   | 31:2W:59:GLU:OE1  | 2.30                     | 0.47              |
| 33:2Y:76:LYS:HD3  | 33:2Y:98:GLU:OE1  | 2.15                     | 0.47              |
| 47:2m:4:C:O2      | 47:2m:4:C:H2'     | 2.14                     | 0.47              |
| 47:2m:85:A:O2'    | 47:2m:149:A:H2'   | 2.14                     | 0.47              |
| 47:2m:216:C:C2'   | 47:2m:217:A:H5'   | 2.45                     | 0.47              |
| 47:2m:222:U:O2'   | 47:2m:223:C:H5'   | 2.14                     | 0.47              |
| 47:2m:352:U:H2'   | 47:2m:353:C:C6    | 2.50                     | 0.47              |
| 47:2m:444:G:N2    | 47:2m:446:G:H3'   | 2.29                     | 0.47              |
| 47:2m:481:C:H5''  | 47:2m:482:G:OP2   | 2.14                     | 0.47              |
| 47:2m:514:U:H2'   | 47:2m:515:G:H5'   | 1.96                     | 0.47              |
| 47:2m:733:C:H2'   | 47:2m:734:C:N1    | 2.30                     | 0.47              |
| 47:2m:808:A:C2'   | 47:2m:809:A:H5'   | 2.45                     | 0.47              |
| 47:2m:810:A:H3'   | 47:2m:811:A:H5'   | 1.97                     | 0.47              |
| 47:2m:872:A:O2'   | 47:2m:873:G:H8    | 1.97                     | 0.47              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 47:2m:1243:U:H2'     | 47:2m:1244:U:O4'   | 2.15                     | 0.47              |
| 47:2m:1265:A:N3      | 47:2m:1265:A:H2'   | 2.30                     | 0.47              |
| 47:2m:1390:U:H2'     | 47:2m:1391:C:H6    | 1.80                     | 0.47              |
| 47:2m:1402:A:H1'     | 62:21:54:VAL:CG2   | 2.43                     | 0.47              |
| 47:2m:1445:U:O2'     | 47:2m:1446:A:H5'   | 2.15                     | 0.47              |
| 47:2m:1518:C:OP2     | 47:2m:1519:U:C6    | 2.67                     | 0.47              |
| 47:2m:1534:C:O2'     | 47:2m:1599:U:O4    | 2.14                     | 0.47              |
| 47:2m:1656:G:C2      | 47:2m:1657:G:C8    | 3.02                     | 0.47              |
| 47:2m:1867:U:H1'     | 47:2m:1868:U:C5    | 2.50                     | 0.47              |
| 48:2n:78:SER:CB      | 48:2n:87:VAL:HG11  | 2.44                     | 0.47              |
| 49:2o:48:LEU:HD12    | 49:2o:48:LEU:O     | 2.15                     | 0.47              |
| 49:2o:65:ARG:HH12    | 74:3L:51:GLU:HG3   | 1.80                     | 0.47              |
| 49:2o:124:HIS:HB3    | 49:2o:138:PHE:CD2  | 2.49                     | 0.47              |
| 50:2p:54:ARG:HG2     | 50:2p:57:ASN:H     | 1.79                     | 0.47              |
| 50:2p:70:THR:HG22    | 50:2p:86:LEU:HG    | 1.97                     | 0.47              |
| 50:2p:71:ALA:HB3     | 55:2u:20:VAL:CG2   | 2.44                     | 0.47              |
| 50:2p:113:LEU:HD23   | 50:2p:118:ALA:CB   | 2.43                     | 0.47              |
| 50:2p:116:ARG:O      | 50:2p:120:TYR:HD1  | 1.98                     | 0.47              |
| 52:2r:34:SER:HB3     | 66:3D:55:VAL:O     | 2.15                     | 0.47              |
| 52:2r:77:MET:HE1     | 52:2r:84:GLY:CA    | 2.45                     | 0.47              |
| 52:2r:165:ASN:HD21   | 52:2r:167:LYS:HD2  | 1.79                     | 0.47              |
| 53:2s:73:GLN:HB3     | 53:2s:135:PHE:CE1  | 2.49                     | 0.47              |
| 53:2s:134:VAL:HG12   | 53:2s:173:PHE:CD2  | 2.49                     | 0.47              |
| 53:2s:139:ILE:HG23   | 53:2s:156:VAL:HG13 | 1.97                     | 0.47              |
| 54:2t:40:PRO:HA      | 54:2t:61:ASP:OD2   | 2.15                     | 0.47              |
| 56:2v:35:ARG:NH1     | 56:2v:55:TYR:O     | 2.34                     | 0.47              |
| 58:2x:60:LYS:C       | 58:2x:60:LYS:CD    | 2.88                     | 0.47              |
| 60:2z:124:ARG:HH21   | 60:2z:129:LEU:HD13 | 1.79                     | 0.47              |
| 61:20:52:TRP:HA      | 61:20:55:THR:CG2   | 2.45                     | 0.47              |
| 66:3D:13:ARG:O       | 66:3D:32:VAL:HB    | 2.14                     | 0.47              |
| 66:3D:31:ARG:HB2     | 66:3D:43:ILE:HD11  | 1.97                     | 0.47              |
| 67:3E:36:LEU:HD21    | 67:3E:43:PHE:CD1   | 2.50                     | 0.47              |
| 68:3F:76:GLN:O       | 68:3F:76:GLN:OE1   | 2.32                     | 0.47              |
| 68:3F:215:GLN:HA     | 68:3F:231:ASP:HA   | 1.97                     | 0.47              |
| 70:3H:61:PHE:CD2     | 70:3H:72:ARG:HD2   | 2.50                     | 0.47              |
| 71:3I:138[A]:ARG:HG2 | 71:3I:156:HIS:CD2  | 2.50                     | 0.47              |
| 76:3N:25:ILE:HD11    | 76:3N:57:VAL:HG12  | 1.95                     | 0.47              |
| 76:3N:124:ASN:OD1    | 76:3N:124:ASN:C    | 2.57                     | 0.47              |
| 1:1A:497:G:H4'       | 1:1A:498:C:OP1     | 2.14                     | 0.47              |
| 1:1A:752:G:H3'       | 1:1A:753:C:O2      | 2.14                     | 0.47              |
| 1:1A:1952:G:OP1      | 21:2M:139:ARG:NE   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2078:C:H2'   | 1:1A:2079:G:H8     | 1.79                     | 0.47              |
| 1:1A:2815:A:C4    | 1:1A:2816:G:C8     | 3.03                     | 0.47              |
| 1:1A:3688:U:OP2   | 4:1D:198:ARG:NH2   | 2.43                     | 0.47              |
| 1:1A:3814:U:O2'   | 1:1A:3815:G:H5'    | 2.15                     | 0.47              |
| 1:1A:3890:A:N7    | 1:1A:4571:A:H1'    | 2.30                     | 0.47              |
| 1:1A:3937:C:OP2   | 1:1A:3938:G:O2'    | 2.29                     | 0.47              |
| 1:1A:3965:A:N1    | 1:1A:4039:G:H5''   | 2.30                     | 0.47              |
| 1:1A:4182:G:H4'   | 4:1D:226:ARG:NH2   | 2.30                     | 0.47              |
| 1:1A:4186:A:H2'   | 1:1A:4187:G:H8     | 1.79                     | 0.47              |
| 1:1A:4296:U:H2'   | 1:1A:4297:G:O4'    | 2.15                     | 0.47              |
| 1:1A:4750:G:H3'   | 1:1A:4751:G:N2     | 2.24                     | 0.47              |
| 2:1B:103:A:H2'    | 2:1B:103:A:N3      | 2.29                     | 0.47              |
| 2:1B:119:U:OP2    | 2:1B:120:U:O2'     | 2.30                     | 0.47              |
| 6:1F:252:TRP:CZ3  | 6:1F:260:LEU:HD11  | 2.50                     | 0.47              |
| 13:2E:36:ALA:HA   | 13:2E:39:VAL:CG1   | 2.45                     | 0.47              |
| 14:2F:81:LEU:HD11 | 14:2F:98:VAL:CG2   | 2.40                     | 0.47              |
| 14:2F:210:LYS:O   | 14:2F:211:LYS:HB2  | 2.14                     | 0.47              |
| 19:2K:178:ARG:O   | 29:2U:51:GLY:HA2   | 2.14                     | 0.47              |
| 21:2M:48:VAL:HG13 | 21:2M:54:MET:HB3   | 1.96                     | 0.47              |
| 26:2R:151:ASN:OD1 | 26:2R:156:ILE:HG21 | 2.15                     | 0.47              |
| 31:2W:106:ARG:HE  | 31:2W:106:ARG:H    | 1.62                     | 0.47              |
| 34:2Z:106:TYR:O   | 34:2Z:108:SER:N    | 2.48                     | 0.47              |
| 38:2d:19:CYS:SG   | 38:2d:21:ARG:O     | 2.73                     | 0.47              |
| 39:2e:8:ILE:O     | 39:2e:12:LEU:HD22  | 2.15                     | 0.47              |
| 40:2f:16:LYS:HD2  | 40:2f:49:LEU:CD2   | 2.45                     | 0.47              |
| 44:2j:26:VAL:HG13 | 44:2j:30:GLU:HG3   | 1.96                     | 0.47              |
| 44:2j:84:ARG:HG2  | 44:2j:88:GLU:OE2   | 2.14                     | 0.47              |
| 47:2m:168:C:H2'   | 47:2m:169:U:H5'    | 1.97                     | 0.47              |
| 47:2m:664:A:O2'   | 47:2m:670:A:N1     | 2.42                     | 0.47              |
| 47:2m:835:C:H42   | 76:3N:9:THR:CG2    | 2.28                     | 0.47              |
| 47:2m:1307:U:H3   | 80:3R:135:HIS:CE1  | 2.33                     | 0.47              |
| 48:2n:120:ARG:NH1 | 69:3G:267:GLN:HB2  | 2.29                     | 0.47              |
| 50:2p:55:THR:C    | 50:2p:58:VAL:HG12  | 2.40                     | 0.47              |
| 50:2p:59:LEU:HD23 | 50:2p:66:ILE:HB    | 1.96                     | 0.47              |
| 50:2p:71:ALA:HB3  | 55:2u:20:VAL:HG21  | 1.96                     | 0.47              |
| 52:2r:56:TYR:CG   | 52:2r:66:CYS:HB2   | 2.50                     | 0.47              |
| 52:2r:164:ARG:C   | 77:3O:41:ARG:HH22  | 2.23                     | 0.47              |
| 60:2z:33:ILE:CG2  | 60:2z:36:VAL:HB    | 2.45                     | 0.47              |
| 69:3G:60:TRP:O    | 69:3G:71:LYS:HE3   | 2.15                     | 0.47              |
| 77:3O:47:LEU:HD22 | 77:3O:79:ILE:CG2   | 2.42                     | 0.47              |
| 78:3P:21:LYS:O    | 78:3P:22:LYS:HB2   | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:308:G:O6      | 16:2H:12:ARG:NH1   | 2.48                     | 0.47              |
| 1:1A:1354:A:H5'    | 19:2K:108:ARG:NH2  | 2.30                     | 0.47              |
| 1:1A:2262:G:N3     | 1:1A:2262:G:H2'    | 2.29                     | 0.47              |
| 1:1A:2669:C:O2'    | 1:1A:2670:C:P      | 2.73                     | 0.47              |
| 1:1A:2757:A:O2'    | 1:1A:2758:G:H5'    | 2.15                     | 0.47              |
| 1:1A:2894:A:H2'    | 1:1A:2895:A:C8     | 2.50                     | 0.47              |
| 1:1A:4108:G:O3'    | 1:1A:4109:G:C8     | 2.68                     | 0.47              |
| 1:1A:4168:G:H2'    | 1:1A:4169:G:H5'    | 1.97                     | 0.47              |
| 1:1A:4760:G:H2'    | 1:1A:4761:G:C8     | 2.50                     | 0.47              |
| 1:1A:4868:G:H2'    | 1:1A:4869:U:C5'    | 2.43                     | 0.47              |
| 3:1C:110:U:O2'     | 3:1C:111:U:H4'     | 2.15                     | 0.47              |
| 8:1H:222:LEU:N     | 8:1H:237:LYS:HE3   | 2.30                     | 0.47              |
| 14:2F:80:GLU:HG2   | 14:2F:110:LEU:CD1  | 2.44                     | 0.47              |
| 16:2H:116:LEU:HD22 | 16:2H:135:ILE:HD11 | 1.96                     | 0.47              |
| 17:2I:58:LEU:HD23  | 17:2I:72:HIS:CG    | 2.50                     | 0.47              |
| 20:2L:81:ARG:HB3   | 20:2L:88:ARG:CZ    | 2.45                     | 0.47              |
| 20:2L:187:THR:O    | 20:2L:188:LEU:HB2  | 2.15                     | 0.47              |
| 21:2M:45:TRP:CD1   | 21:2M:56:LYS:HG3   | 2.50                     | 0.47              |
| 23:2O:38:ASN:HA    | 23:2O:41:GLN:CG    | 2.44                     | 0.47              |
| 28:2T:29:ILE:HG13  | 28:2T:40:HIS:CE1   | 2.50                     | 0.47              |
| 46:2I:104:ALA:C    | 46:2I:105:LYS:HD2  | 2.40                     | 0.47              |
| 47:2m:49:C:H2'     | 47:2m:472:C:H41    | 1.80                     | 0.47              |
| 47:2m:170:A:O2'    | 47:2m:171:A:H5'    | 2.15                     | 0.47              |
| 47:2m:432:G:H2'    | 47:2m:433:A:H8     | 1.78                     | 0.47              |
| 47:2m:650:A:OP2    | 64:3B:108:LYS:HG2  | 2.15                     | 0.47              |
| 47:2m:669:A:H3'    | 47:2m:669:A:P      | 2.54                     | 0.47              |
| 47:2m:1056:U:C2'   | 47:2m:1057:C:H5'   | 2.45                     | 0.47              |
| 47:2m:1124:C:H5''  | 49:2o:150:ILE:HG13 | 1.97                     | 0.47              |
| 47:2m:1261:C:O2    | 67:3E:10:HIS:NE2   | 2.46                     | 0.47              |
| 47:2m:1266:C:O2'   | 47:2m:1267:C:H5'   | 2.15                     | 0.47              |
| 47:2m:1369:A:O2'   | 47:2m:1370:A:H5'   | 2.14                     | 0.47              |
| 47:2m:1606:G:H5''  | 61:20:86:GLY:CA    | 2.44                     | 0.47              |
| 47:2m:1610:G:H2'   | 47:2m:1611:G:N9    | 2.28                     | 0.47              |
| 48:2n:23:THR:HG22  | 48:2n:23:THR:O     | 2.15                     | 0.47              |
| 50:2p:98:ALA:HA    | 50:2p:188:ILE:CD1  | 2.45                     | 0.47              |
| 51:2q:183:VAL:O    | 51:2q:189:LEU:HD12 | 2.15                     | 0.47              |
| 52:2r:103:LEU:HD11 | 77:3O:67:LEU:HB2   | 1.96                     | 0.47              |
| 58:2x:42:ILE:HD12  | 58:2x:42:ILE:HA    | 1.78                     | 0.47              |
| 58:2x:85:ARG:HH22  | 58:2x:118:THR:HG23 | 1.79                     | 0.47              |
| 59:2y:60:ARG:HG3   | 59:2y:63:ARG:NE    | 2.28                     | 0.47              |
| 60:2z:40:TYR:O     | 60:2z:43:VAL:HG13  | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:3F:217:MET:HB3  | 68:3F:229:THR:OG1  | 2.14                     | 0.47              |
| 68:3F:228:TYR:CE2  | 68:3F:230:LEU:HB3  | 2.50                     | 0.47              |
| 1:1A:930:G:OP1     | 6:1F:353:LYS:HE3   | 2.15                     | 0.47              |
| 1:1A:1314:C:C2     | 1:1A:1315:C:C5     | 3.03                     | 0.47              |
| 1:1A:1404:G:H2'    | 1:1A:1404:G:N3     | 2.29                     | 0.47              |
| 1:1A:1440:U:H2'    | 1:1A:1441:C:C6     | 2.50                     | 0.47              |
| 1:1A:1743:A:N1     | 1:1A:1789:C:O2'    | 2.48                     | 0.47              |
| 1:1A:2407:G:OP2    | 1:1A:2407:G:N2     | 2.42                     | 0.47              |
| 1:1A:2835:A:O2'    | 5:1E:228:TYR:O     | 2.32                     | 0.47              |
| 1:1A:3659:G:OP1    | 4:1D:241:ARG:HG2   | 2.15                     | 0.47              |
| 1:1A:3667:C:H4'    | 4:1D:7:GLY:O       | 2.14                     | 0.47              |
| 1:1A:3974:G:N2     | 1:1A:4050:A:H8     | 2.13                     | 0.47              |
| 1:1A:4271:A:H3'    | 1:1A:4272:G:N2     | 2.29                     | 0.47              |
| 1:1A:4624:A:H5'    | 5:1E:223:THR:HG21  | 1.97                     | 0.47              |
| 1:1A:4724:A:H2'    | 1:1A:4725:C:O4'    | 2.15                     | 0.47              |
| 2:1B:3:C:H2'       | 2:1B:4:U:H6        | 1.80                     | 0.47              |
| 3:1C:66:A:H2'      | 3:1C:67:U:C6       | 2.50                     | 0.47              |
| 3:1C:125:C:H4'     | 3:1C:125:C:OP1     | 2.14                     | 0.47              |
| 4:1D:28:ARG:HB2    | 4:1D:123:ARG:CB    | 2.39                     | 0.47              |
| 12:2D:187:LYS:HE3  | 12:2D:187:LYS:HB3  | 1.71                     | 0.47              |
| 16:2H:146:PRO:O    | 16:2H:147:ASP:HB2  | 2.15                     | 0.47              |
| 18:2J:94:MET:CG    | 18:2J:148:MET:HE3  | 2.34                     | 0.47              |
| 39:2e:19:ASP:OD1   | 39:2e:19:ASP:N     | 2.47                     | 0.47              |
| 44:2j:52:VAL:HG13  | 44:2j:52:VAL:O     | 2.14                     | 0.47              |
| 46:2l:53:VAL:HG11  | 46:2l:185:LEU:HD13 | 1.97                     | 0.47              |
| 47:2m:95:G:H21     | 47:2m:474:G:C4'    | 2.27                     | 0.47              |
| 47:2m:681:U:P      | 64:3B:8:ARG:HH21   | 2.38                     | 0.47              |
| 48:2n:187:GLY:HA2  | 63:3A:45:ARG:NE    | 2.29                     | 0.47              |
| 50:2p:51:LEU:HB3   | 50:2p:91:VAL:CG1   | 2.45                     | 0.47              |
| 50:2p:60:GLY:H     | 50:2p:65:ARG:HB2   | 1.77                     | 0.47              |
| 50:2p:75:LYS:HD2   | 55:2u:22:VAL:N     | 2.30                     | 0.47              |
| 51:2q:103:TYR:CD2  | 51:2q:189:LEU:HD11 | 2.50                     | 0.47              |
| 58:2x:17:LYS:HA    | 58:2x:126:ARG:CZ   | 2.45                     | 0.47              |
| 64:3B:131:LEU:HD21 | 64:3B:135:LYS:HE2  | 1.96                     | 0.47              |
| 65:3C:45:VAL:CG2   | 65:3C:64:LEU:HB3   | 2.45                     | 0.47              |
| 68:3F:217:MET:CB   | 68:3F:229:THR:HG23 | 2.45                     | 0.47              |
| 69:3G:137:VAL:HG22 | 69:3G:217:ALA:HA   | 1.97                     | 0.47              |
| 70:3H:23:LYS:HD3   | 70:3H:41:LEU:CB    | 2.44                     | 0.47              |
| 73:3K:37:ILE:HG22  | 73:3K:75:LEU:HD21  | 1.96                     | 0.47              |
| 75:3M:36:ARG:NH1   | 75:3M:39:THR:OG1   | 2.48                     | 0.47              |
| 1:1A:15:A:H2'      | 1:1A:16:G:O4'      | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:40:G:N2       | 1:1A:4380:A:H62    | 2.13                     | 0.46              |
| 1:1A:262:G:H2'     | 1:1A:263:G:H8      | 1.80                     | 0.46              |
| 1:1A:935:A:H1'     | 15:2G:44:GLN:HB3   | 1.97                     | 0.46              |
| 1:1A:1194:G:O2'    | 1:1A:1195:G:H5'    | 2.15                     | 0.46              |
| 1:1A:1444:G:H2'    | 1:1A:1444:G:N3     | 2.30                     | 0.46              |
| 1:1A:1983:A:O2'    | 1:1A:1984:A:H5'    | 2.15                     | 0.46              |
| 1:1A:2333:G:C2'    | 1:1A:2334:C:H5'    | 2.45                     | 0.46              |
| 1:1A:2335:C:H2'    | 1:1A:2336:G:H8     | 1.80                     | 0.46              |
| 1:1A:2574:G:OP2    | 28:2T:67:LYS:NZ    | 2.27                     | 0.46              |
| 1:1A:2602:G:H2'    | 1:1A:2603:C:C6     | 2.50                     | 0.46              |
| 1:1A:3668:C:H5'    | 4:1D:8:GLN:O       | 2.15                     | 0.46              |
| 1:1A:3670:C:O2'    | 1:1A:3671:G:C8     | 2.67                     | 0.46              |
| 1:1A:3883:U:H2'    | 1:1A:3884:U:C6     | 2.50                     | 0.46              |
| 1:1A:3972:A:H8     | 1:1A:4041:C:C5     | 2.33                     | 0.46              |
| 1:1A:4368:G:OP1    | 81:1A:5118:84D:O6  | 2.33                     | 0.46              |
| 1:1A:4507:A:H2'    | 1:1A:4508:C:H6     | 1.80                     | 0.46              |
| 3:1C:132:G:H2'     | 3:1C:133:G:H8      | 1.80                     | 0.46              |
| 4:1D:5:ILE:HG22    | 4:1D:208:GLU:O     | 2.15                     | 0.46              |
| 5:1E:29:VAL:O      | 5:1E:30:LYS:HB2    | 2.14                     | 0.46              |
| 5:1E:285:TYR:N     | 5:1E:332:MET:O     | 2.47                     | 0.46              |
| 6:1F:308:LYS:HD3   | 6:1F:310:HIS:NE2   | 2.30                     | 0.46              |
| 7:1G:65:ALA:HB2    | 7:1G:74:ILE:HD13   | 1.97                     | 0.46              |
| 12:2D:46:PHE:HE1   | 12:2D:141:LYS:HD2  | 1.80                     | 0.46              |
| 15:2G:25:VAL:CG2   | 15:2G:38:VAL:HG13  | 2.45                     | 0.46              |
| 17:2I:77:SER:HB2   | 17:2I:104:VAL:HG23 | 1.96                     | 0.46              |
| 22:2N:107:LYS:HZ2  | 22:2N:107:LYS:C    | 2.23                     | 0.46              |
| 23:2O:19:LEU:HB3   | 23:2O:74:SER:H     | 1.79                     | 0.46              |
| 37:2c:46:GLU:HA    | 37:2c:46:GLU:OE1   | 2.15                     | 0.46              |
| 46:2l:116:LEU:CD2  | 46:2l:116:LEU:H    | 2.28                     | 0.46              |
| 47:2m:321:C:H2'    | 47:2m:322:C:H1'    | 1.97                     | 0.46              |
| 47:2m:821:G:C2     | 71:3I:150:ARG:HG3  | 2.50                     | 0.46              |
| 47:2m:934:G:N7     | 81:2m:1903:84D:N2  | 2.64                     | 0.46              |
| 47:2m:1046:U:H2'   | 47:2m:1047:C:C6    | 2.50                     | 0.46              |
| 47:2m:1199:A:H2'   | 47:2m:1200:A:H8    | 1.76                     | 0.46              |
| 47:2m:1596:U:H2'   | 47:2m:1597:C:H5'   | 1.97                     | 0.46              |
| 48:2n:75:SER:HB2   | 48:2n:122:LEU:HD12 | 1.97                     | 0.46              |
| 50:2p:177:LEU:HD23 | 50:2p:178:ARG:N    | 2.29                     | 0.46              |
| 57:2w:74:GLU:HG2   | 57:2w:75:VAL:N     | 2.30                     | 0.46              |
| 59:2y:109:LEU:HG   | 59:2y:111:PHE:CE1  | 2.49                     | 0.46              |
| 60:2z:44:VAL:HG21  | 60:2z:71:MET:HE3   | 1.97                     | 0.46              |
| 70:3H:16:ILE:HD12  | 70:3H:17:GLU:N     | 2.29                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:457:G:H5'     | 8:1H:115:TYR:HD2   | 1.78                     | 0.46              |
| 1:1A:517:C:N4      | 1:1A:646:G:O2'     | 2.48                     | 0.46              |
| 1:1A:674:G:H2'     | 1:1A:675:C:H6      | 1.78                     | 0.46              |
| 1:1A:2775:C:H2'    | 1:1A:2776:G:C8     | 2.50                     | 0.46              |
| 1:1A:4041:C:O2'    | 46:2l:101:LYS:HD3  | 2.15                     | 0.46              |
| 4:1D:2:GLY:HA2     | 4:1D:207:VAL:HG23  | 1.95                     | 0.46              |
| 7:1G:86:TYR:HE1    | 7:1G:247:ILE:HG13  | 1.77                     | 0.46              |
| 10:2B:105:GLU:HB2  | 10:2B:109:GLU:HG3  | 1.97                     | 0.46              |
| 15:2G:24:LEU:HD11  | 15:2G:86:TRP:CG    | 2.50                     | 0.46              |
| 19:2K:39:THR:HG23  | 19:2K:132:LYS:HD3  | 1.96                     | 0.46              |
| 25:2Q:78:PHE:HE2   | 70:3H:8:PRO:HB2    | 1.77                     | 0.46              |
| 28:2T:22:LYS:HD3   | 28:2T:129:TRP:CZ3  | 2.50                     | 0.46              |
| 46:2l:65:VAL:HG13  | 46:2l:110:PHE:C    | 2.40                     | 0.46              |
| 47:2m:613:G:H1     | 47:2m:629:A:P      | 2.37                     | 0.46              |
| 47:2m:1037:G:H4'   | 47:2m:1845:A:H4'   | 1.97                     | 0.46              |
| 47:2m:1407:U:H3    | 47:2m:1440:C:N4    | 2.13                     | 0.46              |
| 47:2m:1513:C:C2'   | 47:2m:1514:G:H8    | 2.26                     | 0.46              |
| 47:2m:1566:G:O6    | 61:20:101:ARG:NH1  | 2.45                     | 0.46              |
| 49:2o:201:CYS:HB2  | 49:2o:207:LEU:HD12 | 1.96                     | 0.46              |
| 50:2p:8:LYS:O      | 50:2p:12:VAL:HG13  | 2.15                     | 0.46              |
| 52:2r:120:GLY:O    | 52:2r:146:ARG:NH2  | 2.49                     | 0.46              |
| 53:2s:159:ASP:O    | 53:2s:160:LYS:HB3  | 2.15                     | 0.46              |
| 54:2t:145:ILE:HA   | 54:2t:148:LYS:HG2  | 1.96                     | 0.46              |
| 56:2v:22:ARG:C     | 56:2v:22:ARG:HD3   | 2.40                     | 0.46              |
| 58:2x:96:TYR:CD1   | 58:2x:100:VAL:HG21 | 2.51                     | 0.46              |
| 60:2z:117:ILE:HG23 | 60:2z:119:ALA:H    | 1.80                     | 0.46              |
| 64:3B:88:ASP:OD2   | 79:3Q:13:ARG:HB2   | 2.15                     | 0.46              |
| 64:3B:105:PHE:HB3  | 64:3B:112:VAL:HG21 | 1.98                     | 0.46              |
| 65:3C:22:ARG:NE    | 65:3C:27:ALA:O     | 2.21                     | 0.46              |
| 68:3F:87:LEU:HB2   | 68:3F:101:PHE:HD2  | 1.80                     | 0.46              |
| 69:3G:63:VAL:O     | 69:3G:64:THR:HG23  | 2.14                     | 0.46              |
| 73:3K:119:GLU:OE2  | 73:3K:141:TYR:HE2  | 1.98                     | 0.46              |
| 73:3K:150:VAL:HG22 | 73:3K:151:ALA:H    | 1.80                     | 0.46              |
| 74:3L:13:GLN:HG2   | 74:3L:13:GLN:O     | 2.15                     | 0.46              |
| 1:1A:69:A:O2'      | 1:1A:70:A:H5'      | 2.15                     | 0.46              |
| 1:1A:130:C:H2'     | 1:1A:131:C:N1      | 2.29                     | 0.46              |
| 1:1A:759:G:P       | 11:2C:50:LYS:HZ3   | 2.38                     | 0.46              |
| 1:1A:1070:G:O2'    | 1:1A:1071:C:H6     | 1.99                     | 0.46              |
| 1:1A:1294:A:O2'    | 1:1A:1295:C:O5'    | 2.27                     | 0.46              |
| 1:1A:1609:U:H2'    | 1:1A:1610:C:O4'    | 2.16                     | 0.46              |
| 1:1A:1660:U:OP1    | 29:2U:15:VAL:HA    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1717:C:O2'   | 1:1A:1718:C:H5'    | 2.15                     | 0.46              |
| 1:1A:1767:A:H62   | 57:2w:10:ARG:HG2   | 1.81                     | 0.46              |
| 1:1A:2389:A:H2'   | 1:1A:2390:G:H8     | 1.80                     | 0.46              |
| 1:1A:2749:C:H2'   | 1:1A:2750:G:H8     | 1.80                     | 0.46              |
| 1:1A:2882:A:C2'   | 1:1A:2883:G:H5'    | 2.45                     | 0.46              |
| 1:1A:4120:U:H3'   | 1:1A:4121:G:C5'    | 2.42                     | 0.46              |
| 1:1A:4251:A:O2'   | 1:1A:4252:C:H5'    | 2.15                     | 0.46              |
| 1:1A:4582:C:H2'   | 1:1A:4583:C:O4'    | 2.15                     | 0.46              |
| 1:1A:4593:C:H2'   | 1:1A:4594:U:H6     | 1.80                     | 0.46              |
| 1:1A:4911:A:OP1   | 5:1E:97:ARG:NH2    | 2.48                     | 0.46              |
| 3:1C:27:U:H2'     | 3:1C:28:C:C6       | 2.50                     | 0.46              |
| 4:1D:46:LYS:HE3   | 4:1D:46:LYS:HB3    | 1.56                     | 0.46              |
| 7:1G:60:ILE:CD1   | 7:1G:93:THR:HA     | 2.44                     | 0.46              |
| 11:2C:92:MET:CE   | 11:2C:161:ILE:HG12 | 2.45                     | 0.46              |
| 25:2Q:101:ARG:NH1 | 25:2Q:101:ARG:HB3  | 2.31                     | 0.46              |
| 26:2R:73:HIS:ND1  | 26:2R:115:LYS:HG2  | 2.30                     | 0.46              |
| 36:2b:5:LYS:O     | 36:2b:9:LEU:HG     | 2.15                     | 0.46              |
| 47:2m:92:A:O2'    | 51:2q:4:GLY:HA3    | 2.15                     | 0.46              |
| 47:2m:164:A:H2'   | 47:2m:165:G:N3     | 2.30                     | 0.46              |
| 47:2m:188:C:N4    | 47:2m:212:C:H42    | 2.12                     | 0.46              |
| 47:2m:222:U:H2'   | 47:2m:223:C:H6     | 1.80                     | 0.46              |
| 47:2m:351:G:H2'   | 47:2m:351:G:N3     | 2.30                     | 0.46              |
| 47:2m:374:G:H2'   | 47:2m:375:U:H6     | 1.78                     | 0.46              |
| 47:2m:653:A:H2'   | 47:2m:654:A:O4'    | 2.14                     | 0.46              |
| 47:2m:1092:G:O2'  | 47:2m:1093:A:H5'   | 2.16                     | 0.46              |
| 47:2m:1180:C:H2'  | 47:2m:1181:A:C8    | 2.51                     | 0.46              |
| 47:2m:1429:G:P    | 58:2x:33:LYS:HZ3   | 2.38                     | 0.46              |
| 47:2m:1801:A:H2'  | 47:2m:1802:C:H6    | 1.80                     | 0.46              |
| 49:2o:97:LEU:HB3  | 49:2o:232:HIS:NE2  | 2.29                     | 0.46              |
| 52:2r:193:LYS:HB3 | 52:2r:193:LYS:HE3  | 1.62                     | 0.46              |
| 54:2t:141:ARG:CG  | 54:2t:145:ILE:HD11 | 2.45                     | 0.46              |
| 55:2u:35:LEU:HD23 | 55:2u:37:ASP:H     | 1.79                     | 0.46              |
| 57:2w:54:HIS:HA   | 57:2w:57:LEU:CD1   | 2.44                     | 0.46              |
| 58:2x:17:LYS:HB3  | 58:2x:126:ARG:HA   | 1.98                     | 0.46              |
| 59:2y:109:LEU:HG  | 59:2y:111:PHE:CD1  | 2.50                     | 0.46              |
| 61:20:16:ARG:NH1  | 61:20:16:ARG:HG3   | 2.31                     | 0.46              |
| 65:3C:45:VAL:HG21 | 65:3C:64:LEU:CB    | 2.45                     | 0.46              |
| 68:3F:30:MET:HG2  | 68:3F:31:ILE:N     | 2.29                     | 0.46              |
| 69:3G:114:LYS:HG2 | 69:3G:121:ARG:CG   | 2.45                     | 0.46              |
| 69:3G:199:PRO:HG3 | 71:3I:58:ARG:HD3   | 1.96                     | 0.46              |
| 72:3J:47:ALA:O    | 72:3J:74:ILE:HD11  | 2.15                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 72:3J:53:ALA:HA    | 72:3J:79:VAL:CG2  | 2.46                     | 0.46              |
| 76:3N:13:MET:HE2   | 76:3N:15:ASN:HB3  | 1.97                     | 0.46              |
| 1:1A:306:A:H2'     | 1:1A:307:A:C8     | 2.51                     | 0.46              |
| 1:1A:457:G:H2'     | 1:1A:458:C:C6     | 2.50                     | 0.46              |
| 1:1A:982:U:O2'     | 1:1A:983:C:H5'    | 2.16                     | 0.46              |
| 1:1A:1181:C:C3'    | 1:1A:1182:C:H5'   | 2.44                     | 0.46              |
| 1:1A:1315:C:H2'    | 1:1A:1316:G:H8    | 1.81                     | 0.46              |
| 1:1A:1959:U:OP2    | 1:1A:1961:G:H1'   | 2.15                     | 0.46              |
| 1:1A:2323:C:H2'    | 1:1A:2324:C:H6    | 1.79                     | 0.46              |
| 1:1A:2496:G:O2'    | 1:1A:2497:C:H5'   | 2.15                     | 0.46              |
| 1:1A:2639:U:H1'    | 35:2a:26:PRO:CA   | 2.46                     | 0.46              |
| 1:1A:4096:C:H2'    | 1:1A:4097:G:O4'   | 2.15                     | 0.46              |
| 1:1A:4604:G:OP1    | 11:2C:174:LYS:NZ  | 2.48                     | 0.46              |
| 1:1A:4933:C:H2'    | 1:1A:4934:A:C8    | 2.51                     | 0.46              |
| 3:1C:130:C:H2'     | 3:1C:131:G:H8     | 1.79                     | 0.46              |
| 5:1E:242:ARG:HA    | 5:1E:248:LEU:HD21 | 1.97                     | 0.46              |
| 6:1F:322:LEU:O     | 6:1F:326:LEU:HG   | 2.16                     | 0.46              |
| 8:1H:190:HIS:HB3   | 8:1H:193:PHE:HD1  | 1.80                     | 0.46              |
| 9:2A:37:PHE:CE1    | 9:2A:41:MET:HE3   | 2.51                     | 0.46              |
| 9:2A:182:TYR:CE2   | 9:2A:203:GLU:HG2  | 2.49                     | 0.46              |
| 13:2E:31:ASP:C     | 13:2E:34:THR:HG22 | 2.41                     | 0.46              |
| 13:2E:49:VAL:HG13  | 13:2E:71:HIS:CE1  | 2.51                     | 0.46              |
| 21:2M:13:VAL:HG22  | 21:2M:29:ARG:HB2  | 1.97                     | 0.46              |
| 27:2S:131:GLU:O    | 27:2S:134:LYS:HG3 | 2.15                     | 0.46              |
| 35:2a:112:GLN:HA   | 35:2a:112:GLN:OE1 | 2.16                     | 0.46              |
| 46:2l:32:VAL:HG13  | 46:2l:169:VAL:CG2 | 2.41                     | 0.46              |
| 46:2l:62:LYS:HD3   | 46:2l:152:LYS:O   | 2.14                     | 0.46              |
| 47:2m:378:U:H2'    | 47:2m:379:C:C6    | 2.51                     | 0.46              |
| 47:2m:396:U:C4'    | 54:2t:14:THR:HG22 | 2.45                     | 0.46              |
| 47:2m:454:U:H2'    | 47:2m:455:A:H8    | 1.81                     | 0.46              |
| 47:2m:1034:A:C2    | 47:2m:1035:A:H1'  | 2.51                     | 0.46              |
| 47:2m:1406:G:H2'   | 47:2m:1407:U:C1'  | 2.45                     | 0.46              |
| 47:2m:1541:G:H1'   | 61:20:12:GLN:HG2  | 1.96                     | 0.46              |
| 48:2n:146:ALA:HB3  | 48:2n:157:VAL:CG1 | 2.45                     | 0.46              |
| 50:2p:123:LEU:HD11 | 50:2p:154:ASP:OD2 | 2.15                     | 0.46              |
| 51:2q:9:LEU:HB2    | 51:2q:30:ARG:HD3  | 1.98                     | 0.46              |
| 52:2r:125:SER:HB2  | 52:2r:135:ARG:HB2 | 1.97                     | 0.46              |
| 55:2u:13:GLU:HG3   | 55:2u:14:LEU:H    | 1.81                     | 0.46              |
| 55:2u:25:LYS:HD3   | 55:2u:46:MET:CE   | 2.13                     | 0.46              |
| 55:2u:32:HIS:NE2   | 55:2u:45:VAL:HG11 | 2.29                     | 0.46              |
| 56:2v:19:ASN:OD1   | 56:2v:19:ASN:N    | 2.48                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:2x:89:SER:HB3   | 58:2x:112:LEU:HD13 | 1.97                     | 0.46              |
| 68:3F:41:ILE:HG22  | 68:3F:43:TRP:NE1   | 2.31                     | 0.46              |
| 68:3F:114:SER:HB3  | 68:3F:156:PHE:CD2  | 2.50                     | 0.46              |
| 68:3F:166:VAL:HB   | 68:3F:176:VAL:HG23 | 1.96                     | 0.46              |
| 71:3I:60:LEU:CB    | 71:3I:94:LEU:HD21  | 2.45                     | 0.46              |
| 76:3N:54:VAL:C     | 76:3N:55:ILE:HD12  | 2.41                     | 0.46              |
| 80:3R:103:LEU:HD12 | 80:3R:105:TYR:CZ   | 2.50                     | 0.46              |
| 1:1A:1806:G:H2'    | 1:1A:1807:C:H6     | 1.79                     | 0.46              |
| 1:1A:2786:C:H5''   | 1:1A:2787:A:C5'    | 2.34                     | 0.46              |
| 1:1A:4084:G:O6     | 4:1D:70:LYS:HE3    | 2.15                     | 0.46              |
| 1:1A:4378:A:O2'    | 1:1A:4379:A:H2'    | 2.16                     | 0.46              |
| 1:1A:4986:G:O2'    | 1:1A:4987:C:H5'    | 2.15                     | 0.46              |
| 3:1C:21:C:C2'      | 3:1C:22:U:H5'      | 2.45                     | 0.46              |
| 7:1G:6:VAL:HG23    | 7:1G:6:VAL:O       | 2.16                     | 0.46              |
| 7:1G:126:THR:HG22  | 7:1G:128:ASP:HB2   | 1.97                     | 0.46              |
| 8:1H:177:GLY:O     | 8:1H:178:PRO:C     | 2.58                     | 0.46              |
| 14:2F:101:ARG:HA   | 37:2c:25:ARG:NH2   | 2.31                     | 0.46              |
| 17:2I:108:ILE:HD12 | 17:2I:160:ARG:CZ   | 2.46                     | 0.46              |
| 25:2Q:94:ARG:NH1   | 70:3H:144:LEU:O    | 2.47                     | 0.46              |
| 28:2T:89:ILE:HD12  | 28:2T:91:LEU:HD13  | 1.94                     | 0.46              |
| 36:2b:16:GLU:OE1   | 36:2b:16:GLU:CA    | 2.63                     | 0.46              |
| 38:2d:34:CYS:HB3   | 38:2d:39:TYR:H     | 1.79                     | 0.46              |
| 46:2l:67:VAL:O     | 46:2l:67:VAL:HG13  | 2.14                     | 0.46              |
| 47:2m:94:G:HO2'    | 47:2m:508:A:HO2'   | 1.50                     | 0.46              |
| 47:2m:126:G:H1     | 70:3H:196:LYS:HD2  | 1.80                     | 0.46              |
| 47:2m:337:C:H3'    | 47:2m:338:G:C5'    | 2.46                     | 0.46              |
| 47:2m:969:U:O4'    | 47:2m:971:G:H1'    | 2.16                     | 0.46              |
| 47:2m:1309:C:N4    | 80:3R:100:LEU:HD21 | 2.30                     | 0.46              |
| 47:2m:1347:U:H2'   | 47:2m:1348:G:H8    | 1.79                     | 0.46              |
| 52:2r:167:LYS:HD3  | 52:2r:172:CYS:SG   | 2.56                     | 0.46              |
| 54:2t:107:THR:OG1  | 54:2t:108:PRO:HD3  | 2.15                     | 0.46              |
| 54:2t:205:ARG:HG3  | 54:2t:205:ARG:NH1  | 2.31                     | 0.46              |
| 55:2u:34:GLU:HG2   | 55:2u:35:LEU:N     | 2.30                     | 0.46              |
| 57:2w:56:LEU:CG    | 57:2w:60:LEU:HD21  | 2.43                     | 0.46              |
| 59:2y:74:GLN:O     | 59:2y:74:GLN:HG2   | 2.16                     | 0.46              |
| 61:20:110:LEU:O    | 61:20:112:MET:HE2  | 2.16                     | 0.46              |
| 67:3E:30:LEU:C     | 67:3E:31:ILE:HD12  | 2.41                     | 0.46              |
| 68:3F:212:LYS:CA   | 68:3F:235:ILE:HG13 | 2.45                     | 0.46              |
| 70:3H:159:ARG:CZ   | 70:3H:171:THR:HG23 | 2.46                     | 0.46              |
| 78:3P:40:CYS:SG    | 78:3P:59:CYS:HB2   | 2.55                     | 0.46              |
| 1:1A:92:C:C2       | 29:2U:55:LYS:HD2   | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1083:U:O2     | 1:1A:1217:G:N2     | 2.49                     | 0.46              |
| 1:1A:1322:A:C6     | 1:1A:1326:A:C8     | 3.04                     | 0.46              |
| 1:1A:1779:U:H2'    | 1:1A:1780:A:H8     | 1.80                     | 0.46              |
| 1:1A:1962:A:OP2    | 1:1A:2023:C:N4     | 2.49                     | 0.46              |
| 1:1A:2375:A:H2'    | 1:1A:2376:A:H8     | 1.80                     | 0.46              |
| 1:1A:2890:C:H2'    | 1:1A:2891:U:C6     | 2.51                     | 0.46              |
| 1:1A:3757:G:H1     | 1:1A:3766:A:H62    | 1.64                     | 0.46              |
| 1:1A:4107:G:H2'    | 1:1A:4108:G:H8     | 1.80                     | 0.46              |
| 1:1A:4215:C:C2     | 1:1A:4216:G:C8     | 3.03                     | 0.46              |
| 1:1A:4243:C:O2     | 1:1A:4243:C:H2'    | 2.15                     | 0.46              |
| 1:1A:4281:A:H2'    | 1:1A:4282:A:H2'    | 1.97                     | 0.46              |
| 3:1C:86:U:H3'      | 36:2b:5:LYS:HZ2    | 1.80                     | 0.46              |
| 11:2C:27:VAL:HG12  | 11:2C:84:VAL:HG21  | 1.98                     | 0.46              |
| 11:2C:59:LYS:HD2   | 11:2C:59:LYS:HA    | 1.70                     | 0.46              |
| 13:2E:82:ILE:HG22  | 13:2E:130:PHE:CE2  | 2.51                     | 0.46              |
| 23:2O:23:LEU:HD13  | 23:2O:39:PHE:CE2   | 2.50                     | 0.46              |
| 25:2Q:68:GLN:HG2   | 70:3H:31:ARG:NH2   | 2.30                     | 0.46              |
| 46:2l:91:LYS:HB2   | 46:2l:91:LYS:HE2   | 1.58                     | 0.46              |
| 47:2m:81:U:C2'     | 47:2m:82:G:H5'     | 2.46                     | 0.46              |
| 47:2m:84:A:H4'     | 76:3N:119:GLY:O    | 2.15                     | 0.46              |
| 47:2m:203:G:H2'    | 47:2m:204:G:C8     | 2.51                     | 0.46              |
| 47:2m:344:U:H2'    | 47:2m:345:U:H6     | 1.81                     | 0.46              |
| 47:2m:948:C:H2'    | 47:2m:949:G:H8     | 1.80                     | 0.46              |
| 47:2m:1238:U:O2'   | 57:2w:126:VAL:HG13 | 2.15                     | 0.46              |
| 47:2m:1473:G:H21   | 47:2m:1475:G:H2'   | 1.81                     | 0.46              |
| 47:2m:1522:A:N7    | 57:2w:128:HIS:HE1  | 2.13                     | 0.46              |
| 47:2m:1823:A:C2'   | 47:2m:1824:A:H5'   | 2.45                     | 0.46              |
| 48:2n:8:LEU:HA     | 48:2n:191:ARG:NH2  | 2.31                     | 0.46              |
| 48:2n:40:LYS:NZ    | 59:2y:101:ASP:OD2  | 2.47                     | 0.46              |
| 48:2n:145:ILE:HG12 | 48:2n:159:ILE:HB   | 1.98                     | 0.46              |
| 50:2p:98:ALA:N     | 50:2p:169:ASP:OD2  | 2.36                     | 0.46              |
| 54:2t:148:LYS:HA   | 54:2t:151:GLU:HG3  | 1.96                     | 0.46              |
| 56:2v:25:LEU:H     | 56:2v:25:LEU:HD13  | 1.80                     | 0.46              |
| 58:2x:54:PRO:HD2   | 58:2x:88:ILE:HD11  | 1.98                     | 0.46              |
| 58:2x:55:VAL:HA    | 58:2x:63:PHE:HE2   | 1.78                     | 0.46              |
| 59:2y:32:LYS:HB2   | 59:2y:51:ALA:CB    | 2.45                     | 0.46              |
| 60:2z:15:VAL:C     | 60:2z:16:LEU:HD12  | 2.40                     | 0.46              |
| 60:2z:46:ARG:HD3   | 60:2z:46:ARG:N     | 2.30                     | 0.46              |
| 66:3D:13:ARG:NH1   | 66:3D:33:GLU:OE2   | 2.49                     | 0.46              |
| 68:3F:168:CYS:HB2  | 68:3F:195:LEU:CD1  | 2.42                     | 0.46              |
| 68:3F:199:THR:HG22 | 68:3F:241:PHE:HD2  | 1.81                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:3G:137:VAL:HG23 | 69:3G:165:VAL:CG2  | 2.45                     | 0.46              |
| 70:3H:212:LEU:HD12 | 70:3H:212:LEU:O    | 2.15                     | 0.46              |
| 71:3I:125:HIS:NE2  | 71:3I:129:LEU:HD21 | 2.31                     | 0.46              |
| 76:3N:41:ARG:HB2   | 76:3N:55:ILE:CG2   | 2.46                     | 0.46              |
| 1:1A:500:G:H1'     | 1:1A:504:G:C3'     | 2.46                     | 0.46              |
| 1:1A:996:G:H1      | 1:1A:1047:C:N4     | 2.13                     | 0.46              |
| 1:1A:1358:G:O2'    | 1:1A:1360:G:O6     | 2.29                     | 0.46              |
| 1:1A:1668:A:C2'    | 1:1A:1669:A:H5'    | 2.46                     | 0.46              |
| 1:1A:1927:U:OP1    | 1:1A:1949:U:O2'    | 2.29                     | 0.46              |
| 1:1A:1980:U:O5'    | 1:1A:1982:G:H5''   | 2.15                     | 0.46              |
| 1:1A:2763:U:H2'    | 1:1A:2764:A:H8     | 1.79                     | 0.46              |
| 1:1A:2861:C:H2'    | 1:1A:2862:G:O4'    | 2.16                     | 0.46              |
| 1:1A:2904:U:O4     | 1:1A:3592:G:H1'    | 2.16                     | 0.46              |
| 1:1A:4742:G:H2'    | 1:1A:4743:G:H8     | 1.79                     | 0.46              |
| 1:1A:4896:G:HO2'   | 1:1A:4897:G:P      | 2.39                     | 0.46              |
| 1:1A:5011:A:O2'    | 1:1A:5012:G:H5'    | 2.16                     | 0.46              |
| 4:1D:114:CYS:HB3   | 4:1D:167:GLY:O     | 2.16                     | 0.46              |
| 6:1F:138:MET:HE2   | 6:1F:138:MET:HB3   | 1.90                     | 0.46              |
| 6:1F:289:LEU:HB2   | 45:2k:4:HIS:CD2    | 2.50                     | 0.46              |
| 7:1G:64:ILE:O      | 7:1G:75:VAL:HG12   | 2.15                     | 0.46              |
| 7:1G:92:LEU:O      | 7:1G:93:THR:HG22   | 2.16                     | 0.46              |
| 7:1G:202:GLN:NE2   | 7:1G:202:GLN:HA    | 2.31                     | 0.46              |
| 13:2E:87:LEU:HD11  | 13:2E:166:PHE:HE1  | 1.79                     | 0.46              |
| 33:2Y:81:ASN:HA    | 33:2Y:111:ILE:HD11 | 1.98                     | 0.46              |
| 39:2e:10:ASP:O     | 39:2e:13:LEU:HG    | 2.14                     | 0.46              |
| 47:2m:559:G:O2'    | 71:3I:173:VAL:HG12 | 2.16                     | 0.46              |
| 47:2m:575:A:C2     | 47:2m:576:A:H1'    | 2.50                     | 0.46              |
| 47:2m:1286:G:N1    | 47:2m:1312:G:O2'   | 2.44                     | 0.46              |
| 47:2m:1410:C:H2'   | 47:2m:1411:G:C8    | 2.51                     | 0.46              |
| 47:2m:1454:A:H61   | 47:2m:1476:A:C5'   | 2.28                     | 0.46              |
| 47:2m:1459:G:OP2   | 68:3F:280:LYS:HD2  | 2.15                     | 0.46              |
| 48:2n:3:GLY:HA3    | 48:2n:8:LEU:CD1    | 2.46                     | 0.46              |
| 48:2n:84:GLN:HA    | 48:2n:87:VAL:HG22  | 1.97                     | 0.46              |
| 51:2q:192:ILE:CD1  | 51:2q:243:GLY:HA3  | 2.46                     | 0.46              |
| 52:2r:35:LEU:HD22  | 52:2r:117:ILE:HD13 | 1.97                     | 0.46              |
| 53:2s:49:LYS:HD2   | 53:2s:179:LYS:NZ   | 2.30                     | 0.46              |
| 54:2t:45:THR:HG22  | 54:2t:55:TYR:CD2   | 2.51                     | 0.46              |
| 54:2t:81:VAL:HG22  | 54:2t:102:VAL:HG12 | 1.98                     | 0.46              |
| 58:2x:12:VAL:HG21  | 58:2x:90:LYS:HB3   | 1.97                     | 0.46              |
| 58:2x:57:LEU:HD21  | 58:2x:111:ILE:HG22 | 1.96                     | 0.46              |
| 64:3B:124:LYS:HA   | 64:3B:128:VAL:O    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 68:3F:27:PHE:HB2  | 68:3F:30:MET:CE    | 2.27                     | 0.46              |
| 68:3F:217:MET:HA  | 68:3F:229:THR:HA   | 1.98                     | 0.46              |
| 71:3I:15:THR:HG23 | 71:3I:16:PRO:HD2   | 1.97                     | 0.46              |
| 71:3I:122:SER:HB3 | 71:3I:125:HIS:HB3  | 1.97                     | 0.46              |
| 73:3K:93:LYS:CB   | 73:3K:150:VAL:HG21 | 2.46                     | 0.46              |
| 75:3M:70:ASN:N    | 75:3M:70:ASN:OD1   | 2.49                     | 0.46              |
| 76:3N:22:GLN:OE1  | 76:3N:74:MET:HE1   | 2.16                     | 0.46              |
| 76:3N:23:MET:SD   | 76:3N:25:ILE:HG13  | 2.55                     | 0.46              |
| 1:1A:139:G:H2'    | 1:1A:140:G:N9      | 2.31                     | 0.46              |
| 1:1A:654:C:O2     | 1:1A:654:C:H2'     | 2.16                     | 0.46              |
| 1:1A:966:A:C2     | 1:1A:2093:A:H2     | 2.34                     | 0.46              |
| 1:1A:1074:G:N3    | 1:1A:1074:G:H2'    | 2.31                     | 0.46              |
| 1:1A:1196:G:H2'   | 1:1A:1197:C:O4'    | 2.16                     | 0.46              |
| 1:1A:1218:G:H5''  | 1:1A:1219:G:OP2    | 2.15                     | 0.46              |
| 1:1A:1613:A:N7    | 1:1A:3638:G:H1'    | 2.31                     | 0.46              |
| 1:1A:1722:C:O2'   | 1:1A:1723:A:H5'    | 2.15                     | 0.46              |
| 1:1A:2054:U:OP2   | 17:2I:44:SER:OG    | 2.19                     | 0.46              |
| 1:1A:2485:U:P     | 1:1A:2486:G:H5'    | 2.56                     | 0.46              |
| 1:1A:4199:C:C2'   | 1:1A:4200:G:H5'    | 2.45                     | 0.46              |
| 3:1C:154:G:H2'    | 3:1C:155:C:H6      | 1.80                     | 0.46              |
| 8:1H:50:LEU:HD23  | 8:1H:54:ILE:O      | 2.15                     | 0.46              |
| 11:2C:51:LYS:HD3  | 11:2C:51:LYS:N     | 2.24                     | 0.46              |
| 21:2M:127:MET:HA  | 22:2N:153:PRO:HD2  | 1.98                     | 0.46              |
| 23:2O:47:ILE:O    | 23:2O:53:ALA:HA    | 2.15                     | 0.46              |
| 29:2U:27:LYS:HA   | 29:2U:27:LYS:HD2   | 1.68                     | 0.46              |
| 45:2k:107:ARG:O   | 45:2k:111:ILE:HG12 | 2.15                     | 0.46              |
| 47:2m:129:C:H5'   | 47:2m:214:U:C2     | 2.51                     | 0.46              |
| 47:2m:218:U:O2'   | 47:2m:219:U:H5'    | 2.16                     | 0.46              |
| 47:2m:329:G:H2'   | 47:2m:330:G:N9     | 2.30                     | 0.46              |
| 47:2m:352:U:O2    | 56:2v:71:ARG:NE    | 2.46                     | 0.46              |
| 47:2m:373:G:OP1   | 56:2v:137:THR:OG1  | 2.23                     | 0.46              |
| 47:2m:429:C:H4'   | 51:2q:12:VAL:CG1   | 2.45                     | 0.46              |
| 47:2m:640:A:H5''  | 71:3I:25:LEU:HD13  | 1.98                     | 0.46              |
| 47:2m:955:A:H61   | 47:2m:971:G:C2'    | 2.24                     | 0.46              |
| 47:2m:1447:G:P    | 62:2I:87:ARG:HH21  | 2.38                     | 0.46              |
| 48:2n:198:MET:HE1 | 59:2y:86:PRO:O     | 2.16                     | 0.46              |
| 50:2p:25:LEU:HD12 | 50:2p:37:VAL:HG11  | 1.97                     | 0.46              |
| 50:2p:54:ARG:HD3  | 50:2p:57:ASN:ND2   | 2.31                     | 0.46              |
| 50:2p:147:ALA:O   | 50:2p:148:LYS:HE2  | 2.15                     | 0.46              |
| 52:2r:19:LEU:N    | 52:2r:23:TRP:O     | 2.48                     | 0.46              |
| 53:2s:15:LYS:HZ1  | 53:2s:17:ASP:HB2   | 1.81                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:2s:149:ASP:OD1 | 53:2s:149:ASP:C    | 2.58                     | 0.46              |
| 56:2v:40:ILE:CD1  | 56:2v:143:LEU:HD23 | 2.45                     | 0.46              |
| 57:2w:34:MET:CE   | 57:2w:45:LEU:HB2   | 2.46                     | 0.46              |
| 57:2w:123:TYR:OH  | 60:2z:124:ARG:NH1  | 2.49                     | 0.46              |
| 58:2x:21:ALA:HB1  | 58:2x:72:VAL:HG22  | 1.98                     | 0.46              |
| 59:2y:56:HIS:HA   | 59:2y:59:LYS:CE    | 2.44                     | 0.46              |
| 61:20:38:LYS:NZ   | 61:20:41:LYS:HB2   | 2.31                     | 0.46              |
| 65:3C:46:GLU:CD   | 74:3L:113:GLN:HB3  | 2.38                     | 0.46              |
| 71:3I:128:VAL:O   | 71:3I:132:GLN:HG3  | 2.16                     | 0.46              |
| 72:3J:53:ALA:HA   | 72:3J:79:VAL:HG23  | 1.98                     | 0.46              |
| 73:3K:20:ARG:HB3  | 73:3K:65:PHE:CE1   | 2.51                     | 0.46              |
| 75:3M:14:ILE:HG22 | 75:3M:72:CYS:SG    | 2.56                     | 0.46              |
| 1:1A:495:C:O2'    | 1:1A:496:G:H5'     | 2.15                     | 0.46              |
| 1:1A:500:G:H1'    | 1:1A:504:G:C2'     | 2.46                     | 0.46              |
| 1:1A:1242:G:H21   | 30:2V:120:ARG:HH12 | 1.64                     | 0.46              |
| 1:1A:1854:G:N2    | 1:1A:4394:A:O4'    | 2.49                     | 0.46              |
| 1:1A:2521:G:H2'   | 1:1A:2522:G:C8     | 2.50                     | 0.46              |
| 1:1A:2526:C:H2'   | 1:1A:2527:A:C8     | 2.51                     | 0.46              |
| 1:1A:2534:C:C2'   | 1:1A:2535:G:H5'    | 2.45                     | 0.46              |
| 1:1A:2552:G:OP2   | 1:1A:2553:A:O2'    | 2.16                     | 0.46              |
| 1:1A:2573:A:H2'   | 1:1A:2574:G:O4'    | 2.15                     | 0.46              |
| 1:1A:2706:G:H2'   | 1:1A:2707:U:C5'    | 2.46                     | 0.46              |
| 1:1A:4092:G:H2'   | 1:1A:4093:G:H5'    | 1.98                     | 0.46              |
| 1:1A:4604:G:N2    | 1:1A:4607:A:OP2    | 2.41                     | 0.46              |
| 1:1A:5047:C:O2'   | 1:1A:5050:C:OP2    | 2.28                     | 0.46              |
| 3:1C:86:U:O2'     | 3:1C:87:G:OP2      | 2.27                     | 0.46              |
| 3:1C:142:U:H2'    | 3:1C:143:G:O4'     | 2.16                     | 0.46              |
| 6:1F:7:LEU:HD23   | 6:1F:23:THR:HA     | 1.96                     | 0.46              |
| 21:2M:19:THR:OG1  | 21:2M:20:PRO:HD2   | 2.16                     | 0.46              |
| 21:2M:83:ARG:HG2  | 21:2M:125:GLN:HB3  | 1.98                     | 0.46              |
| 25:2Q:106:GLU:OE1 | 25:2Q:106:GLU:HA   | 2.15                     | 0.46              |
| 25:2Q:119:LYS:HE3 | 25:2Q:119:LYS:HB3  | 1.64                     | 0.46              |
| 29:2U:93:ASN:OD1  | 29:2U:93:ASN:C     | 2.58                     | 0.46              |
| 42:2h:1:MET:HE3   | 47:2m:1851:A:H5'   | 1.97                     | 0.46              |
| 47:2m:28:U:H2'    | 47:2m:29:G:H8      | 1.81                     | 0.46              |
| 47:2m:546:G:H2'   | 47:2m:546:G:N3     | 2.31                     | 0.46              |
| 47:2m:962:A:O2'   | 47:2m:963:A:H5'    | 2.15                     | 0.46              |
| 47:2m:969:U:H4'   | 47:2m:971:G:H1'    | 1.97                     | 0.46              |
| 47:2m:986:G:O4'   | 74:3L:138:ASP:HB2  | 2.15                     | 0.46              |
| 47:2m:1453:C:HO2' | 47:2m:1454:A:P     | 2.33                     | 0.46              |
| 47:2m:1601:A:H4'  | 47:2m:1602:U:H5''  | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1687:C:N3    | 47:2m:1688:C:C5    | 2.84                     | 0.46              |
| 47:2m:1711:U:H2'   | 47:2m:1712:A:H8    | 1.80                     | 0.46              |
| 48:2n:157:VAL:HG11 | 48:2n:160:ALA:HB2  | 1.98                     | 0.46              |
| 50:2p:9:ARG:O      | 50:2p:12:VAL:HG22  | 2.16                     | 0.46              |
| 52:2r:139:VAL:HG22 | 52:2r:140:ASP:O    | 2.16                     | 0.46              |
| 54:2t:8:TRP:O      | 54:2t:18:ARG:HD3   | 2.16                     | 0.46              |
| 58:2x:11:GLN:OE1   | 58:2x:71:ARG:NH1   | 2.49                     | 0.46              |
| 58:2x:39:LEU:H     | 58:2x:39:LEU:HD22  | 1.80                     | 0.46              |
| 59:2y:46:LEU:CD1   | 59:2y:50:ILE:HD11  | 2.44                     | 0.46              |
| 59:2y:99:ASP:HB2   | 59:2y:100:PRO:HD2  | 1.98                     | 0.46              |
| 60:2z:40:TYR:HA    | 60:2z:43:VAL:CG1   | 2.46                     | 0.46              |
| 64:3B:32:LEU:HG    | 64:3B:34:THR:H     | 1.80                     | 0.46              |
| 64:3B:36:LEU:HD13  | 64:3B:36:LEU:C     | 2.41                     | 0.46              |
| 68:3F:191:HIS:NE2  | 68:3F:195:LEU:HD21 | 2.31                     | 0.46              |
| 68:3F:212:LYS:HG3  | 68:3F:235:ILE:HG12 | 1.98                     | 0.46              |
| 72:3J:30:GLY:C     | 72:3J:31:LEU:HD23  | 2.40                     | 0.46              |
| 77:3O:47:LEU:HD11  | 77:3O:50:PHE:HD2   | 1.80                     | 0.46              |
| 80:3R:135:HIS:CE1  | 80:3R:140:TYR:HB3  | 2.51                     | 0.46              |
| 1:1A:60:G:H2'      | 1:1A:61:A:H8       | 1.79                     | 0.46              |
| 1:1A:136:C:O5'     | 1:1A:137:G:H5'     | 2.15                     | 0.46              |
| 1:1A:518:G:N1      | 1:1A:643:C:H2'     | 2.31                     | 0.46              |
| 1:1A:1080:C:H5''   | 1:1A:1081:C:OP2    | 2.15                     | 0.46              |
| 1:1A:1098:G:H2'    | 1:1A:1099:C:C5     | 2.51                     | 0.46              |
| 1:1A:1346:C:OP1    | 19:2K:148:VAL:HG12 | 2.16                     | 0.46              |
| 1:1A:1816:C:O2     | 1:1A:1816:C:H2'    | 2.15                     | 0.46              |
| 1:1A:1837:A:OP2    | 22:2N:130:ARG:NH1  | 2.40                     | 0.46              |
| 1:1A:2633:U:H2'    | 1:1A:2634:C:H6     | 1.81                     | 0.46              |
| 1:1A:2767:U:H3'    | 1:1A:2769:U:C6     | 2.51                     | 0.46              |
| 1:1A:4139:G:H2'    | 1:1A:4140:C:O4'    | 2.15                     | 0.46              |
| 1:1A:4327:C:HO2'   | 1:1A:4328:G:H5'    | 1.81                     | 0.46              |
| 1:1A:4480:A:H2'    | 1:1A:4481:U:O4'    | 2.16                     | 0.46              |
| 1:1A:4487:A:O2'    | 1:1A:4708:A:N1     | 2.45                     | 0.46              |
| 1:1A:4606:G:H2'    | 1:1A:4607:A:O4'    | 2.15                     | 0.46              |
| 1:1A:5027:C:O5'    | 54:2t:77:ARG:NH2   | 2.49                     | 0.46              |
| 2:1B:7:G:OP1       | 7:1G:33:ARG:HD2    | 2.16                     | 0.46              |
| 7:1G:154:THR:HG23  | 7:1G:155:THR:N     | 2.31                     | 0.46              |
| 10:2B:151:LYS:HE2  | 10:2B:151:LYS:HA   | 1.97                     | 0.46              |
| 11:2C:115:ARG:HG2  | 11:2C:123:ILE:HG12 | 1.97                     | 0.46              |
| 16:2H:184:ILE:O    | 16:2H:184:ILE:HG12 | 2.16                     | 0.46              |
| 21:2M:2:LYS:O      | 21:2M:121:ALA:HB3  | 2.16                     | 0.46              |
| 24:2P:18:LEU:HD13  | 24:2P:54:ALA:O     | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:299:A:O2'    | 47:2m:300:U:H5'    | 2.16                     | 0.46              |
| 47:2m:452:G:H2'    | 47:2m:453:C:H6     | 1.81                     | 0.46              |
| 47:2m:1139:C:H5    | 47:2m:1149:A:H62   | 1.64                     | 0.46              |
| 47:2m:1435:C:H4'   | 47:2m:1436:C:C6    | 2.51                     | 0.46              |
| 47:2m:1452:A:O4'   | 47:2m:1475:G:N1    | 2.49                     | 0.46              |
| 47:2m:1601:A:H4'   | 47:2m:1602:U:C5'   | 2.46                     | 0.46              |
| 47:2m:1604:G:H2'   | 47:2m:1605:G:C5'   | 2.45                     | 0.46              |
| 47:2m:1681:U:H2'   | 47:2m:1682:C:C6    | 2.50                     | 0.46              |
| 48:2n:85:ARG:NH1   | 48:2n:205:ARG:HD3  | 2.31                     | 0.46              |
| 50:2p:158:ILE:HG13 | 50:2p:164:VAL:HG13 | 1.97                     | 0.46              |
| 50:2p:220:THR:HG23 | 50:2p:221:THR:N    | 2.30                     | 0.46              |
| 52:2r:77:MET:HE3   | 52:2r:77:MET:HB2   | 1.80                     | 0.46              |
| 52:2r:153:LEU:HB3  | 52:2r:189:ALA:CB   | 2.46                     | 0.46              |
| 53:2s:17:ASP:HA    | 53:2s:20:GLU:HG3   | 1.97                     | 0.46              |
| 53:2s:51:ILE:HG21  | 53:2s:179:LYS:HD2  | 1.96                     | 0.46              |
| 53:2s:143:ARG:HB2  | 53:2s:155:LYS:HB2  | 1.98                     | 0.46              |
| 54:2t:11:ARG:HG2   | 54:2t:16:GLY:O     | 2.15                     | 0.46              |
| 54:2t:62:VAL:HG11  | 54:2t:75:LYS:HD2   | 1.98                     | 0.46              |
| 56:2v:15:THR:O     | 56:2v:16:ILE:HD13  | 2.15                     | 0.46              |
| 56:2v:30:LYS:HG2   | 56:2v:31:GLU:N     | 2.29                     | 0.46              |
| 57:2w:108:LYS:CD   | 57:2w:110:GLU:H    | 2.26                     | 0.46              |
| 58:2x:105:LYS:HA   | 58:2x:108:ILE:HG12 | 1.98                     | 0.46              |
| 60:2z:78:LYS:O     | 60:2z:78:LYS:CD    | 2.44                     | 0.46              |
| 61:20:11:GLN:HG3   | 61:20:62:ARG:NH1   | 2.31                     | 0.46              |
| 63:3A:32:ILE:HG12  | 63:3A:60:ARG:HD2   | 1.98                     | 0.46              |
| 65:3C:37:LYS:HG2   | 65:3C:72:HIS:ND1   | 2.31                     | 0.46              |
| 70:3H:23:LYS:CE    | 70:3H:42:GLY:H     | 2.29                     | 0.46              |
| 70:3H:118:GLU:HG2  | 70:3H:119:LYS:N    | 2.30                     | 0.46              |
| 70:3H:218:LYS:HD2  | 70:3H:222:GLU:HG3  | 1.98                     | 0.46              |
| 71:3I:170:PRO:CB   | 71:3I:174:LYS:HD2  | 2.46                     | 0.46              |
| 73:3K:150:VAL:HG22 | 73:3K:151:ALA:N    | 2.31                     | 0.46              |
| 75:3M:24:GLN:NE2   | 75:3M:64:ASN:OD1   | 2.39                     | 0.46              |
| 1:1A:646:G:H2'     | 1:1A:647:G:O4'     | 2.16                     | 0.45              |
| 1:1A:923:C:H2'     | 1:1A:925:C:C5      | 2.47                     | 0.45              |
| 1:1A:1257:A:C2     | 1:1A:1258:G:H1'    | 2.51                     | 0.45              |
| 1:1A:1493:G:H2'    | 1:1A:1494:U:C6     | 2.51                     | 0.45              |
| 1:1A:2295:C:H2'    | 1:1A:2296:G:H8     | 1.80                     | 0.45              |
| 1:1A:2443:G:H2'    | 1:1A:2444:U:O4'    | 2.16                     | 0.45              |
| 1:1A:4065:G:H2'    | 1:1A:4066:U:OP1    | 2.16                     | 0.45              |
| 1:1A:4741:C:N4     | 1:1A:4958:C:H42    | 2.14                     | 0.45              |
| 1:1A:4900:C:H3'    | 1:1A:4900:C:P      | 2.56                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:1C:44:A:H2'      | 3:1C:45:C:C6       | 2.51                     | 0.45              |
| 3:1C:137:A:H2'     | 3:1C:138:C:H6      | 1.81                     | 0.45              |
| 4:1D:95:GLN:HB3    | 44:2j:87:LYS:NZ    | 2.31                     | 0.45              |
| 8:1H:147:GLY:HA3   | 8:1H:203:ILE:HG12  | 1.94                     | 0.45              |
| 9:2A:92:VAL:CG1    | 9:2A:140:ILE:HD12  | 2.46                     | 0.45              |
| 18:2J:122:ALA:HB1  | 18:2J:123:PRO:HD2  | 1.98                     | 0.45              |
| 30:2V:101:HIS:CE1  | 30:2V:104:LEU:HD23 | 2.51                     | 0.45              |
| 31:2W:44:LYS:HE2   | 31:2W:44:LYS:HA    | 1.97                     | 0.45              |
| 32:2X:57:MET:HE2   | 32:2X:88:LEU:CB    | 2.46                     | 0.45              |
| 43:2i:59:LYS:HE3   | 43:2i:59:LYS:HB3   | 1.63                     | 0.45              |
| 43:2i:104:ILE:HG22 | 43:2i:105:GLN:HG2  | 1.98                     | 0.45              |
| 46:2l:112:ALA:HA   | 46:2l:135:PRO:HB2  | 1.98                     | 0.45              |
| 47:2m:5:U:O2'      | 47:2m:6:G:H5'      | 2.16                     | 0.45              |
| 47:2m:208:G:H22    | 54:2t:144:LYS:NZ   | 2.14                     | 0.45              |
| 47:2m:878:G:H2'    | 47:2m:878:G:N3     | 2.30                     | 0.45              |
| 47:2m:996:A:C5'    | 73:3K:7:PRO:HD3    | 2.46                     | 0.45              |
| 47:2m:1261:C:H5'   | 47:2m:1262:C:P     | 2.56                     | 0.45              |
| 47:2m:1402:A:C4'   | 62:21:51:LYS:HE2   | 2.44                     | 0.45              |
| 47:2m:1589:A:H2'   | 47:2m:1590:C:H6    | 1.80                     | 0.45              |
| 47:2m:1864:U:H3'   | 65:3C:5:ARG:NH2    | 2.30                     | 0.45              |
| 48:2n:52:LYS:HZ2   | 63:3A:83:PHE:HA    | 1.80                     | 0.45              |
| 48:2n:77:ILE:CD1   | 48:2n:99:ILE:HD12  | 2.47                     | 0.45              |
| 50:2p:67:ARG:NH1   | 55:2u:93:THR:O     | 2.48                     | 0.45              |
| 51:2q:67:GLN:HB2   | 51:2q:69:PHE:CZ    | 2.51                     | 0.45              |
| 53:2s:15:LYS:H     | 53:2s:16:PRO:HD3   | 1.75                     | 0.45              |
| 54:2t:125:LYS:HB3  | 54:2t:128:LYS:HZ1  | 1.80                     | 0.45              |
| 55:2u:52:LEU:HD23  | 55:2u:58:VAL:HG22  | 1.98                     | 0.45              |
| 56:2v:59:LYS:HA    | 56:2v:66:VAL:HG13  | 1.97                     | 0.45              |
| 56:2v:69:ARG:O     | 56:2v:69:ARG:HG2   | 2.16                     | 0.45              |
| 59:2y:45:LYS:O     | 59:2y:48:ASN:OD1   | 2.34                     | 0.45              |
| 59:2y:126:MET:HA   | 59:2y:128:PHE:CE1  | 2.51                     | 0.45              |
| 65:3C:24:THR:CG2   | 65:3C:72:HIS:H     | 2.30                     | 0.45              |
| 69:3G:251:LEU:HD11 | 69:3G:256:TRP:HD1  | 1.81                     | 0.45              |
| 70:3H:165:GLU:H    | 70:3H:165:GLU:CD   | 2.24                     | 0.45              |
| 72:3J:34:GLY:O     | 72:3J:38:ALA:HB2   | 2.15                     | 0.45              |
| 76:3N:106:GLN:HA   | 76:3N:109:GLU:OE1  | 2.17                     | 0.45              |
| 1:1A:109:G:H5'     | 14:2F:92:ARG:NE    | 2.30                     | 0.45              |
| 1:1A:286:U:H2'     | 1:1A:287:U:H6      | 1.82                     | 0.45              |
| 1:1A:726:G:O2'     | 1:1A:727:C:H5'     | 2.17                     | 0.45              |
| 1:1A:2094:G:N3     | 1:1A:2094:G:C2'    | 2.78                     | 0.45              |
| 1:1A:2297:G:H4'    | 6:1F:242:PRO:HB2   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2463:G:C2'    | 1:1A:2464:C:H5'    | 2.46                     | 0.45              |
| 1:1A:2667:C:O4'    | 20:2L:96:MET:HG3   | 2.16                     | 0.45              |
| 1:1A:2741:U:H2'    | 4:1D:50:HIS:CD2    | 2.51                     | 0.45              |
| 1:1A:2889:G:H2'    | 1:1A:2890:C:H6     | 1.81                     | 0.45              |
| 1:1A:3907:G:H2'    | 1:1A:4447:C:O2'    | 2.15                     | 0.45              |
| 1:1A:3933:G:H2'    | 1:1A:3934:G:H8     | 1.81                     | 0.45              |
| 1:1A:4044:U:H4'    | 1:1A:4045:G:C4     | 2.51                     | 0.45              |
| 1:1A:4281:A:N6     | 1:1A:4283:G:H1'    | 2.30                     | 0.45              |
| 1:1A:4357:G:H2'    | 1:1A:4358:U:H6     | 1.82                     | 0.45              |
| 2:1B:68:C:C2'      | 2:1B:69:U:H5'      | 2.46                     | 0.45              |
| 3:1C:75:G:O2'      | 3:1C:76:C:H5'      | 2.16                     | 0.45              |
| 3:1C:87:G:C1'      | 3:1C:88:A:OP2      | 2.61                     | 0.45              |
| 5:1E:121:ASN:OD1   | 5:1E:124:LYS:HG3   | 2.16                     | 0.45              |
| 6:1F:64:ALA:HB1    | 6:1F:78:ARG:C      | 2.41                     | 0.45              |
| 6:1F:158:VAL:CG2   | 6:1F:170:LEU:HD22  | 2.47                     | 0.45              |
| 12:2D:55:ASP:OD1   | 12:2D:162:ARG:HB3  | 2.17                     | 0.45              |
| 15:2G:126:GLU:OE1  | 15:2G:130:LEU:HD13 | 2.17                     | 0.45              |
| 21:2M:2:LYS:HE2    | 21:2M:35:PRO:HD3   | 1.98                     | 0.45              |
| 24:2P:20:LEU:HD12  | 24:2P:20:LEU:HA    | 1.80                     | 0.45              |
| 28:2T:41:ALA:HB2   | 28:2T:77:TYR:HE1   | 1.81                     | 0.45              |
| 31:2W:106:ARG:HE   | 31:2W:106:ARG:N    | 2.14                     | 0.45              |
| 33:2Y:108:ARG:HD2  | 33:2Y:128:ARG:HG2  | 1.98                     | 0.45              |
| 34:2Z:5:LEU:HD12   | 34:2Z:5:LEU:HA     | 1.82                     | 0.45              |
| 38:2d:60:GLY:HA2   | 38:2d:64:MET:SD    | 2.56                     | 0.45              |
| 38:2d:68:LYS:HG3   | 38:2d:69:ILE:N     | 2.32                     | 0.45              |
| 46:2l:109:ALA:HB3  | 46:2l:156:LYS:NZ   | 2.31                     | 0.45              |
| 47:2m:559:G:N3     | 47:2m:559:G:O4'    | 2.46                     | 0.45              |
| 47:2m:993:G:O2'    | 47:2m:994:C:H5'    | 2.16                     | 0.45              |
| 47:2m:1003:U:H2'   | 47:2m:1004:U:C6    | 2.52                     | 0.45              |
| 47:2m:1101:U:C2    | 47:2m:1102:G:N7    | 2.85                     | 0.45              |
| 47:2m:1208:A:H4'   | 47:2m:1835:A:N7    | 2.31                     | 0.45              |
| 47:2m:1214:A:H2'   | 47:2m:1217:A:N7    | 2.31                     | 0.45              |
| 47:2m:1525:C:H5'   | 47:2m:1526:G:OP1   | 2.16                     | 0.45              |
| 47:2m:1610:G:C6    | 47:2m:1630:A:N1    | 2.84                     | 0.45              |
| 47:2m:1808:U:H2'   | 47:2m:1809:A:C8    | 2.51                     | 0.45              |
| 49:2o:167:LYS:NZ   | 49:2o:200:ALA:HB1  | 2.32                     | 0.45              |
| 54:2t:121:LEU:HD12 | 54:2t:122:GLY:N    | 2.32                     | 0.45              |
| 59:2y:60:ARG:HA    | 59:2y:63:ARG:HE    | 1.81                     | 0.45              |
| 64:3B:84:PHE:CE2   | 64:3B:86:PRO:HB3   | 2.51                     | 0.45              |
| 66:3D:61:SER:C     | 66:3D:62:GLU:HG2   | 2.41                     | 0.45              |
| 69:3G:108:LYS:HB2  | 69:3G:233:LEU:HD13 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 71:3I:170:PRO:HB2 | 71:3I:174:LYS:HD2  | 1.98                     | 0.45              |
| 76:3N:38:THR:O    | 76:3N:42:GLU:HG3   | 2.17                     | 0.45              |
| 76:3N:75:ILE:O    | 76:3N:75:ILE:HG23  | 2.15                     | 0.45              |
| 77:3O:69:THR:H    | 77:3O:72:VAL:CG1   | 2.30                     | 0.45              |
| 79:3Q:35:ARG:HD2  | 79:3Q:39:ASN:HD21  | 1.80                     | 0.45              |
| 1:1A:182:G:H3'    | 1:1A:183:C:H4'     | 1.99                     | 0.45              |
| 1:1A:488:G:H2'    | 1:1A:489:C:O4'     | 2.17                     | 0.45              |
| 1:1A:513:U:N3     | 1:1A:515:C:H5''    | 2.32                     | 0.45              |
| 1:1A:731:G:O2'    | 1:1A:732:A:H5'     | 2.16                     | 0.45              |
| 1:1A:743:G:H2'    | 1:1A:744:G:H1'     | 1.99                     | 0.45              |
| 1:1A:1082:C:H4'   | 1:1A:1083:U:OP1    | 2.17                     | 0.45              |
| 1:1A:1514:U:H2'   | 1:1A:1515:A:C8     | 2.51                     | 0.45              |
| 1:1A:1742:A:OP2   | 7:1G:10:LYS:HE3    | 2.16                     | 0.45              |
| 1:1A:1772:C:C6    | 1:1A:1773:U:H5     | 2.35                     | 0.45              |
| 1:1A:2652:G:C4    | 35:2a:50:PRO:HG3   | 2.51                     | 0.45              |
| 1:1A:2700:G:H2'   | 1:1A:2701:U:C6     | 2.52                     | 0.45              |
| 1:1A:2860:C:H4'   | 1:1A:3837:C:H4'    | 1.98                     | 0.45              |
| 1:1A:3661:G:N7    | 4:1D:152:SER:OG    | 2.43                     | 0.45              |
| 1:1A:3700:C:O4'   | 1:1A:3775:A:H1'    | 2.16                     | 0.45              |
| 1:1A:3707:U:H2'   | 1:1A:3708:C:H6     | 1.81                     | 0.45              |
| 1:1A:3953:G:H2'   | 1:1A:3954:A:C4     | 2.51                     | 0.45              |
| 1:1A:4320:G:H2'   | 1:1A:4321:U:C6     | 2.50                     | 0.45              |
| 1:1A:4704:C:H2'   | 1:1A:4705:A:C8     | 2.51                     | 0.45              |
| 1:1A:4715:C:OP1   | 5:1E:348:ARG:NH2   | 2.49                     | 0.45              |
| 1:1A:5004:C:C2'   | 1:1A:5005:G:H5'    | 2.46                     | 0.45              |
| 2:1B:33:U:O2'     | 2:1B:34:C:P        | 2.74                     | 0.45              |
| 4:1D:49:ILE:HD13  | 4:1D:60:LYS:HE3    | 1.99                     | 0.45              |
| 13:2E:9:GLU:C     | 13:2E:11:PRO:HD2   | 2.41                     | 0.45              |
| 13:2E:10:ASN:N    | 13:2E:11:PRO:HD2   | 2.31                     | 0.45              |
| 13:2E:87:LEU:CD1  | 13:2E:166:PHE:HE1  | 2.30                     | 0.45              |
| 13:2E:175:LEU:CD1 | 13:2E:176:PRO:HD2  | 2.46                     | 0.45              |
| 14:2F:140:SER:HA  | 14:2F:143:GLU:HB2  | 1.98                     | 0.45              |
| 15:2G:119:ARG:O   | 15:2G:123:ILE:HG13 | 2.15                     | 0.45              |
| 29:2U:63:LEU:HD22 | 29:2U:64:LYS:N     | 2.30                     | 0.45              |
| 41:2g:120:ASN:C   | 41:2g:121:LEU:HD23 | 2.41                     | 0.45              |
| 45:2k:57:GLY:O    | 45:2k:58:LYS:HD3   | 2.17                     | 0.45              |
| 45:2k:90:LEU:HD22 | 45:2k:111:ILE:HG23 | 1.98                     | 0.45              |
| 47:2m:151:C:OP1   | 76:3N:120:THR:OG1  | 2.28                     | 0.45              |
| 47:2m:432:G:H2'   | 47:2m:433:A:C8     | 2.52                     | 0.45              |
| 47:2m:520:A:O2'   | 47:2m:825:A:N3     | 2.39                     | 0.45              |
| 47:2m:527:C:H2'   | 47:2m:528:A:C8     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:589:G:O2'   | 47:2m:590:A:H3'    | 2.16                     | 0.45              |
| 47:2m:944:A:H1'   | 74:3L:136:PRO:CB   | 2.34                     | 0.45              |
| 47:2m:1340:U:P    | 47:2m:1341:C:H3'   | 2.56                     | 0.45              |
| 47:2m:1359:U:O2'  | 47:2m:1360:U:H5'   | 2.15                     | 0.45              |
| 47:2m:1361:G:H1'  | 47:2m:1379:A:N7    | 2.31                     | 0.45              |
| 47:2m:1560:U:C2   | 47:2m:1575:G:O6    | 2.69                     | 0.45              |
| 47:2m:1644:C:H2'  | 47:2m:1645:C:C6    | 2.51                     | 0.45              |
| 47:2m:1645:C:H5'' | 58:2x:138:ARG:O    | 2.16                     | 0.45              |
| 47:2m:1648:G:H5'' | 58:2x:125:ARG:CB   | 2.45                     | 0.45              |
| 47:2m:1839:U:H1'  | 47:2m:1863:A:H2    | 1.81                     | 0.45              |
| 48:2n:32:PHE:CE2  | 48:2n:33:GLN:HG3   | 2.52                     | 0.45              |
| 48:2n:34:MET:HE1  | 48:2n:162:PRO:HB2  | 1.97                     | 0.45              |
| 48:2n:105:PRO:HA  | 48:2n:132:GLN:NE2  | 2.30                     | 0.45              |
| 48:2n:123:VAL:HA  | 48:2n:145:ILE:O    | 2.16                     | 0.45              |
| 50:2p:133:GLY:HA3 | 50:2p:156:LEU:O    | 2.17                     | 0.45              |
| 50:2p:164:VAL:O   | 50:2p:164:VAL:CG2  | 2.60                     | 0.45              |
| 51:2q:92:ILE:HG21 | 76:3N:17:LEU:HD11  | 1.98                     | 0.45              |
| 51:2q:121:TYR:CD2 | 51:2q:161:GLN:HG2  | 2.51                     | 0.45              |
| 52:2r:112:LEU:CD1 | 52:2r:177:LEU:HD21 | 2.47                     | 0.45              |
| 53:2s:6:ALA:HB3   | 53:2s:28:LEU:HD22  | 1.99                     | 0.45              |
| 55:2u:7:ASN:OD1   | 55:2u:40:VAL:HG13  | 2.16                     | 0.45              |
| 56:2v:95:TYR:HB2  | 56:2v:102:PHE:CE1  | 2.51                     | 0.45              |
| 57:2w:72:LYS:NZ   | 57:2w:93:MET:HB2   | 2.31                     | 0.45              |
| 58:2x:9:SER:HB2   | 58:2x:24:HIS:NE2   | 2.30                     | 0.45              |
| 59:2y:109:LEU:O   | 59:2y:110:ASP:HB2  | 2.16                     | 0.45              |
| 60:2z:26:ILE:HD12 | 60:2z:26:ILE:O     | 2.16                     | 0.45              |
| 60:2z:47:LYS:CE   | 60:2z:77:TYR:HB3   | 2.46                     | 0.45              |
| 60:2z:55:ARG:HB2  | 60:2z:58:GLU:OE1   | 2.15                     | 0.45              |
| 62:21:22:ILE:HD12 | 62:21:114:VAL:HG12 | 1.97                     | 0.45              |
| 68:3F:178:ASN:OD1 | 68:3F:180:ALA:HB3  | 2.16                     | 0.45              |
| 68:3F:289:LEU:CD1 | 68:3F:298:LEU:HD22 | 2.44                     | 0.45              |
| 72:3J:42:LEU:CD2  | 72:3J:110:VAL:HG21 | 2.35                     | 0.45              |
| 79:3Q:34:ARG:O    | 79:3Q:37:GLN:HG3   | 2.16                     | 0.45              |
| 1:1A:249:C:N3     | 1:1A:250:C:C5      | 2.85                     | 0.45              |
| 1:1A:1348:U:H2'   | 1:1A:1349:G:H8     | 1.82                     | 0.45              |
| 1:1A:1754:U:H2'   | 1:1A:1755:C:H5     | 1.80                     | 0.45              |
| 1:1A:1764:G:H2'   | 1:1A:1766:A:OP2    | 2.16                     | 0.45              |
| 1:1A:1811:G:H2'   | 1:1A:1812:C:H6     | 1.81                     | 0.45              |
| 1:1A:2040:A:H4'   | 1:1A:2041:A:O5'    | 2.16                     | 0.45              |
| 1:1A:2668:G:O2'   | 1:1A:2669:C:H5'    | 2.17                     | 0.45              |
| 1:1A:3971:G:C3'   | 1:1A:3972:A:H5''   | 2.45                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4913:G:H4'    | 1:1A:4914:C:OP2    | 2.15                     | 0.45              |
| 1:1A:5024:C:H41    | 1:1A:5028:G:C2'    | 2.30                     | 0.45              |
| 2:1B:3:C:H2'       | 2:1B:4:U:C6        | 2.52                     | 0.45              |
| 4:1D:14:SER:HA     | 4:1D:17:ARG:HH21   | 1.81                     | 0.45              |
| 4:1D:189:TYR:CD2   | 4:1D:196:TRP:HB2   | 2.51                     | 0.45              |
| 5:1E:223:THR:O     | 5:1E:274:TYR:HA    | 2.17                     | 0.45              |
| 7:1G:86:TYR:OH     | 7:1G:104:LEU:HD13  | 2.17                     | 0.45              |
| 9:2A:53:LYS:HE2    | 9:2A:189:ASP:OD2   | 2.16                     | 0.45              |
| 13:2E:144:LYS:O    | 13:2E:148:THR:HG22 | 2.16                     | 0.45              |
| 15:2G:123:ILE:HD13 | 17:2I:182:GLU:CG   | 2.47                     | 0.45              |
| 23:2O:107:LYS:O    | 23:2O:108:GLU:HG3  | 2.17                     | 0.45              |
| 34:2Z:37:ASP:OD1   | 34:2Z:37:ASP:N     | 2.49                     | 0.45              |
| 46:2l:85:MET:SD    | 46:2l:86:ASP:O     | 2.74                     | 0.45              |
| 47:2m:150:A:N6     | 47:2m:168:C:C4     | 2.83                     | 0.45              |
| 47:2m:294:U:C6     | 56:2v:15:THR:HG21  | 2.52                     | 0.45              |
| 47:2m:524:U:H3'    | 47:2m:525:A:H5'    | 1.99                     | 0.45              |
| 47:2m:821:G:H2'    | 47:2m:824:C:OP1    | 2.16                     | 0.45              |
| 47:2m:1070:A:H2'   | 47:2m:1071:G:O4'   | 2.16                     | 0.45              |
| 47:2m:1304:U:H5'   | 80:3R:95:ARG:HG2   | 1.99                     | 0.45              |
| 47:2m:1453:C:O2    | 47:2m:1453:C:C2'   | 2.65                     | 0.45              |
| 47:2m:1539:U:H2'   | 47:2m:1540:G:H8    | 1.82                     | 0.45              |
| 47:2m:1595:U:O2'   | 47:2m:1596:U:H5'   | 2.16                     | 0.45              |
| 47:2m:1598:G:C2'   | 77:3O:80:ARG:HG2   | 2.46                     | 0.45              |
| 47:2m:1683:C:H2'   | 47:2m:1684:C:C6    | 2.50                     | 0.45              |
| 47:2m:1687:C:C2    | 47:2m:1688:C:C5    | 3.05                     | 0.45              |
| 81:2m:1902:84D:O5  | 81:2m:1902:84D:O6  | 2.35                     | 0.45              |
| 50:2p:178:ARG:HD3  | 50:2p:178:ARG:C    | 2.41                     | 0.45              |
| 51:2q:62:LYS:O     | 51:2q:66:MET:HG2   | 2.16                     | 0.45              |
| 53:2s:142:LYS:HB2  | 75:3M:54:ASP:HB3   | 1.98                     | 0.45              |
| 54:2t:56:ARG:HA    | 54:2t:180:GLY:CA   | 2.46                     | 0.45              |
| 55:2u:19:GLY:O     | 55:2u:71:LEU:HB2   | 2.16                     | 0.45              |
| 58:2x:25:CYS:SG    | 58:2x:66:VAL:HG21  | 2.57                     | 0.45              |
| 58:2x:32:ILE:HG23  | 58:2x:32:ILE:O     | 2.17                     | 0.45              |
| 58:2x:33:LYS:HG2   | 58:2x:38:PRO:HA    | 1.99                     | 0.45              |
| 58:2x:43:GLU:O     | 58:2x:44:PRO:C     | 2.59                     | 0.45              |
| 59:2y:19:LYS:HB2   | 59:2y:20:TYR:CD1   | 2.52                     | 0.45              |
| 62:21:40:ILE:CD1   | 62:21:53:PRO:HG3   | 2.46                     | 0.45              |
| 63:3A:74:LYS:HG2   | 63:3A:81:LYS:HA    | 1.98                     | 0.45              |
| 68:3F:74:ASP:N     | 68:3F:74:ASP:OD1   | 2.49                     | 0.45              |
| 68:3F:258:ILE:HG22 | 68:3F:267:VAL:CB   | 2.43                     | 0.45              |
| 70:3H:144:LEU:HD23 | 70:3H:145:PHE:CD1  | 2.50                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 71:3I:124:HIS:O   | 71:3I:128:VAL:HG23 | 2.15                     | 0.45              |
| 72:3J:18:LEU:O    | 72:3J:21:VAL:HG22  | 2.16                     | 0.45              |
| 78:3P:34:ASP:HA   | 78:3P:44:THR:O     | 2.16                     | 0.45              |
| 1:1A:76:A:H5'     | 14:2F:101:ARG:HH21 | 1.79                     | 0.45              |
| 1:1A:285:G:H2'    | 1:1A:286:U:C6      | 2.51                     | 0.45              |
| 1:1A:287:U:H2'    | 1:1A:288:G:C8      | 2.50                     | 0.45              |
| 1:1A:479:G:H2'    | 1:1A:480:C:H6      | 1.82                     | 0.45              |
| 1:1A:1365:C:O2'   | 1:1A:1366:G:OP1    | 2.24                     | 0.45              |
| 1:1A:1502:G:H2'   | 1:1A:1502:G:N3     | 2.32                     | 0.45              |
| 1:1A:1764:G:H2'   | 1:1A:1766:A:P      | 2.56                     | 0.45              |
| 1:1A:2629:C:O2'   | 1:1A:2630:U:H5'    | 2.16                     | 0.45              |
| 1:1A:2760:G:C1'   | 1:1A:2761:U:OP2    | 2.57                     | 0.45              |
| 1:1A:2793:G:H3'   | 1:1A:2794:C:H5'    | 1.98                     | 0.45              |
| 1:1A:2889:G:O2'   | 1:1A:2890:C:H5'    | 2.17                     | 0.45              |
| 1:1A:3597:G:H2'   | 1:1A:3598:C:H6     | 1.78                     | 0.45              |
| 1:1A:3711:A:H2'   | 1:1A:3711:A:N3     | 2.31                     | 0.45              |
| 1:1A:4288:C:O2'   | 1:1A:4321:U:OP1    | 2.33                     | 0.45              |
| 1:1A:4732:G:H5''  | 1:1A:4733:C:C5'    | 2.46                     | 0.45              |
| 1:1A:4958:C:O2'   | 1:1A:4959:U:H5'    | 2.16                     | 0.45              |
| 2:1B:33:U:H2'     | 2:1B:34:C:H6       | 1.80                     | 0.45              |
| 2:1B:58:A:C2      | 2:1B:59:G:C5       | 3.05                     | 0.45              |
| 6:1F:318:PRO:C    | 6:1F:320:LYS:H     | 2.23                     | 0.45              |
| 7:1G:217:ASP:HA   | 7:1G:220:LYS:CD    | 2.46                     | 0.45              |
| 10:2B:165:GLU:OE1 | 16:2H:26:ARG:NH2   | 2.32                     | 0.45              |
| 15:2G:126:GLU:CG  | 17:2I:185:VAL:HG13 | 2.43                     | 0.45              |
| 19:2K:186:TYR:HE2 | 19:2K:188:ASN:HD22 | 1.64                     | 0.45              |
| 22:2N:42:ILE:CG2  | 22:2N:53:PRO:HG3   | 2.46                     | 0.45              |
| 23:2O:31:ASP:OD1  | 23:2O:31:ASP:C     | 2.59                     | 0.45              |
| 28:2T:29:ILE:HG13 | 28:2T:40:HIS:NE2   | 2.32                     | 0.45              |
| 33:2Y:82:VAL:HG13 | 33:2Y:114:ARG:HG2  | 1.98                     | 0.45              |
| 46:2I:103:LEU:HB3 | 46:2I:106:LYS:HB3  | 1.97                     | 0.45              |
| 47:2m:65:C:C2     | 70:3H:133:LEU:HD22 | 2.52                     | 0.45              |
| 47:2m:94:G:O2'    | 47:2m:508:A:O2'    | 2.25                     | 0.45              |
| 47:2m:157:U:H1'   | 70:3H:59:GLN:O     | 2.16                     | 0.45              |
| 47:2m:445:A:H2'   | 47:2m:446:G:O4'    | 2.17                     | 0.45              |
| 47:2m:1019:C:C2'  | 47:2m:1020:A:H5'   | 2.45                     | 0.45              |
| 47:2m:1189:A:H2'  | 47:2m:1190:A:C8    | 2.51                     | 0.45              |
| 47:2m:1512:C:O2'  | 47:2m:1513:C:H5''  | 2.17                     | 0.45              |
| 51:2q:95:THR:HG23 | 51:2q:97:GLU:OE1   | 2.17                     | 0.45              |
| 51:2q:121:TYR:OH  | 51:2q:235:TRP:O    | 2.35                     | 0.45              |
| 51:2q:181:CYS:HB3 | 51:2q:195:ILE:CD1  | 2.41                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:2r:119:SER:O   | 52:2r:121:PRO:HD3  | 2.17                     | 0.45              |
| 54:2t:130:THR:N   | 54:2t:131:PRO:CD   | 2.80                     | 0.45              |
| 55:2u:16:PHE:CE2  | 55:2u:85:LEU:HD13  | 2.51                     | 0.45              |
| 61:20:31:PRO:HB2  | 61:20:33:TRP:CD1   | 2.51                     | 0.45              |
| 61:20:45:LEU:HD23 | 61:20:45:LEU:HA    | 1.83                     | 0.45              |
| 62:21:100:GLN:HG2 | 62:21:101:ILE:N    | 2.32                     | 0.45              |
| 64:3B:54:LYS:HD3  | 64:3B:91:LEU:HD11  | 1.98                     | 0.45              |
| 65:3C:34:LYS:HG2  | 65:3C:34:LYS:O     | 2.15                     | 0.45              |
| 66:3D:21:THR:CG2  | 66:3D:27:CYS:HB2   | 2.38                     | 0.45              |
| 68:3F:48:ASP:OD1  | 68:3F:51:ASN:HB3   | 2.17                     | 0.45              |
| 70:3H:30:LYS:CD   | 70:3H:36:VAL:HG21  | 2.39                     | 0.45              |
| 77:3O:65:TYR:O    | 77:3O:68:ILE:HD11  | 2.17                     | 0.45              |
| 77:3O:107:VAL:C   | 77:3O:108:ILE:HD12 | 2.41                     | 0.45              |
| 1:1A:248:C:H2'    | 1:1A:249:C:H6      | 1.82                     | 0.45              |
| 1:1A:989:U:H2'    | 1:1A:990:C:C6      | 2.52                     | 0.45              |
| 1:1A:1613:A:H5''  | 4:1D:183:GLY:HA3   | 1.99                     | 0.45              |
| 1:1A:2261:G:C5'   | 8:1H:112:MET:HE2   | 2.42                     | 0.45              |
| 1:1A:2333:G:H5''  | 6:1F:195:LYS:HE3   | 1.99                     | 0.45              |
| 1:1A:2404:A:H3'   | 1:1A:2405:G:H8     | 1.81                     | 0.45              |
| 1:1A:4063:U:H5''  | 1:1A:4064:C:C5     | 2.49                     | 0.45              |
| 1:1A:4079:C:H2'   | 1:1A:4080:C:C6     | 2.51                     | 0.45              |
| 1:1A:4095:G:N2    | 1:1A:4114:C:OP1    | 2.40                     | 0.45              |
| 1:1A:4768:G:OP1   | 17:2I:176:ARG:NH1  | 2.50                     | 0.45              |
| 3:1C:64:U:C2      | 3:1C:65:A:C8       | 3.05                     | 0.45              |
| 8:1H:201:ILE:HD13 | 8:1H:261:ILE:HG12  | 1.99                     | 0.45              |
| 10:2B:106:THR:OG1 | 10:2B:109:GLU:OE2  | 2.26                     | 0.45              |
| 12:2D:48:LEU:O    | 12:2D:139:ARG:HA   | 2.16                     | 0.45              |
| 13:2E:32:ARG:HG2  | 13:2E:126:TYR:HE1  | 1.81                     | 0.45              |
| 19:2K:9:LYS:HD3   | 19:2K:9:LYS:HA     | 1.57                     | 0.45              |
| 23:2O:61:VAL:HG22 | 23:2O:74:SER:HB3   | 1.99                     | 0.45              |
| 26:2R:40:ILE:CG2  | 26:2R:42:THR:HG23  | 2.47                     | 0.45              |
| 34:2Z:33:VAL:O    | 34:2Z:33:VAL:HG22  | 2.16                     | 0.45              |
| 41:2g:93:LYS:HD3  | 41:2g:102:ARG:HG2  | 1.98                     | 0.45              |
| 47:2m:168:C:OP1   | 70:3H:131:ARG:HD3  | 2.15                     | 0.45              |
| 47:2m:512:A:C2    | 47:2m:513:G:C8     | 3.05                     | 0.45              |
| 47:2m:538:U:H2'   | 47:2m:540:U:O4'    | 2.17                     | 0.45              |
| 47:2m:581:U:O2    | 76:3N:33:ALA:HA    | 2.17                     | 0.45              |
| 47:2m:666:U:H2'   | 47:2m:667:U:C6     | 2.51                     | 0.45              |
| 47:2m:805:U:P     | 75:3M:82:GLN:HG2   | 2.57                     | 0.45              |
| 47:2m:941:C:H2'   | 47:2m:942:G:H8     | 1.81                     | 0.45              |
| 47:2m:957:A:O2'   | 47:2m:958:G:N3     | 2.39                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:2m:971:G:H8     | 47:2m:971:G:OP2   | 2.00                     | 0.45              |
| 47:2m:1035:A:C4    | 47:2m:1036:A:C8   | 3.04                     | 0.45              |
| 47:2m:1364:U:H2'   | 47:2m:1365:G:H5'  | 1.97                     | 0.45              |
| 47:2m:1648:G:N2    | 47:2m:1674:G:H2'  | 2.32                     | 0.45              |
| 48:2n:84:GLN:HG2   | 48:2n:100:ALA:HB1 | 1.99                     | 0.45              |
| 50:2p:72:VAL:HG13  | 55:2u:20:VAL:HB   | 1.98                     | 0.45              |
| 50:2p:95:GLY:HA2   | 50:2p:101:GLN:CD  | 2.41                     | 0.45              |
| 51:2q:139:LEU:HD21 | 51:2q:147:ILE:HB  | 1.98                     | 0.45              |
| 54:2t:84:ASN:OD1   | 54:2t:86:SER:OG   | 2.27                     | 0.45              |
| 55:2u:3:MET:HE1    | 55:2u:8:ARG:HD3   | 1.99                     | 0.45              |
| 55:2u:5:LYS:O      | 55:2u:9:ILE:HG13  | 2.16                     | 0.45              |
| 55:2u:92:ALA:HB1   | 55:2u:96:ARG:CG   | 2.47                     | 0.45              |
| 56:2v:61:PRO:HD3   | 56:2v:141:ASN:OD1 | 2.17                     | 0.45              |
| 61:20:130:ASP:O    | 61:20:133:ARG:HG3 | 2.16                     | 0.45              |
| 64:3B:85:VAL:HG11  | 64:3B:94:ILE:HD13 | 1.98                     | 0.45              |
| 65:3C:46:GLU:O     | 65:3C:49:ALA:N    | 2.47                     | 0.45              |
| 66:3D:12:ALA:O     | 66:3D:55:VAL:HG23 | 2.17                     | 0.45              |
| 66:3D:26:GLN:HG2   | 66:3D:27:CYS:N    | 2.30                     | 0.45              |
| 68:3F:69:VAL:HG23  | 68:3F:80:SER:HB3  | 1.99                     | 0.45              |
| 69:3G:101:SER:O    | 69:3G:103:LYS:NZ  | 2.32                     | 0.45              |
| 71:3I:135:ILE:HG22 | 71:3I:136:ARG:N   | 2.32                     | 0.45              |
| 76:3N:35:VAL:CG2   | 76:3N:40:ILE:HG12 | 2.46                     | 0.45              |
| 77:3O:92:LEU:HD21  | 77:3O:109:TYR:CE1 | 2.52                     | 0.45              |
| 80:3R:102:VAL:HG21 | 80:3R:104:LYS:HZ1 | 1.81                     | 0.45              |
| 1:1A:119:G:C5      | 10:2B:132:ARG:HD2 | 2.52                     | 0.45              |
| 1:1A:190:G:H2'     | 1:1A:191:G:C8     | 2.51                     | 0.45              |
| 1:1A:306:A:H2'     | 1:1A:307:A:H8     | 1.81                     | 0.45              |
| 1:1A:1174:G:H21    | 7:1G:275:GLN:NE2  | 2.14                     | 0.45              |
| 1:1A:1207:C:H2'    | 1:1A:1208:G:H8    | 1.81                     | 0.45              |
| 1:1A:1399:G:H2'    | 1:1A:1400:G:C8    | 2.52                     | 0.45              |
| 1:1A:1411:C:O2'    | 1:1A:1412:G:N7    | 2.36                     | 0.45              |
| 1:1A:1563:A:C2     | 47:2m:677:G:H4'   | 2.52                     | 0.45              |
| 1:1A:2009:A:N3     | 1:1A:2009:A:H3'   | 2.32                     | 0.45              |
| 1:1A:2358:G:O2'    | 1:1A:2359:U:H5'   | 2.17                     | 0.45              |
| 1:1A:2904:U:H3     | 1:1A:3592:G:H4'   | 1.81                     | 0.45              |
| 1:1A:4054:C:C2     | 46:2l:207:LYS:HD3 | 2.52                     | 0.45              |
| 1:1A:4079:C:H2'    | 1:1A:4080:C:H6    | 1.82                     | 0.45              |
| 1:1A:4302:U:H2'    | 1:1A:4303:C:H5'   | 1.99                     | 0.45              |
| 1:1A:4539:U:C2'    | 1:1A:4540:C:H5'   | 2.47                     | 0.45              |
| 1:1A:4904:G:C2'    | 1:1A:4905:C:H5'   | 2.46                     | 0.45              |
| 1:1A:4935:C:H2'    | 1:1A:4936:G:H8    | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4991:U:H2'    | 1:1A:4992:G:H8     | 1.82                     | 0.45              |
| 3:1C:39:G:H1'      | 3:1C:103:A:N6      | 2.31                     | 0.45              |
| 3:1C:60:G:O6       | 3:1C:96:C:O2'      | 2.31                     | 0.45              |
| 6:1F:221:PHE:HD2   | 6:1F:227:ILE:HD13  | 1.82                     | 0.45              |
| 8:1H:157:HIS:HB3   | 8:1H:160:LYS:HG3   | 1.99                     | 0.45              |
| 14:2F:127:PHE:HB2  | 36:2b:118:LYS:O    | 2.17                     | 0.45              |
| 15:2G:41:PRO:HB2   | 15:2G:74:ARG:HB2   | 1.98                     | 0.45              |
| 15:2G:126:GLU:OE1  | 15:2G:126:GLU:O    | 2.34                     | 0.45              |
| 21:2M:19:THR:C     | 21:2M:21:LYS:H     | 2.23                     | 0.45              |
| 27:2S:10:ASP:HB3   | 27:2S:13:LYS:HB2   | 1.98                     | 0.45              |
| 29:2U:93:ASN:OD1   | 29:2U:94:LYS:N     | 2.50                     | 0.45              |
| 46:2l:92:LYS:HE2   | 46:2l:92:LYS:N     | 2.31                     | 0.45              |
| 46:2l:162:VAL:HG12 | 46:2l:164:CYS:O    | 2.16                     | 0.45              |
| 47:2m:168:C:H2'    | 47:2m:168:C:O2     | 2.17                     | 0.45              |
| 47:2m:550:C:OP2    | 47:2m:550:C:H6     | 1.99                     | 0.45              |
| 47:2m:560:A:C5'    | 71:3l:174:LYS:HE2  | 2.46                     | 0.45              |
| 47:2m:688:U:H1'    | 47:2m:689:U:OP2    | 2.16                     | 0.45              |
| 47:2m:878:G:C6     | 47:2m:908:A:N1     | 2.81                     | 0.45              |
| 47:2m:903:A:H2'    | 47:2m:904:A:H5''   | 1.99                     | 0.45              |
| 47:2m:916:A:C6     | 73:3K:73:ARG:HD3   | 2.51                     | 0.45              |
| 47:2m:1385:G:OP1   | 50:2p:159:HIS:N    | 2.35                     | 0.45              |
| 47:2m:1616:U:H2'   | 47:2m:1617:G:H8    | 1.79                     | 0.45              |
| 47:2m:1797:U:H2'   | 47:2m:1798:C:H6    | 1.81                     | 0.45              |
| 48:2n:11:LYS:HA    | 48:2n:11:LYS:CE    | 2.46                     | 0.45              |
| 50:2p:75:LYS:CD    | 55:2u:21:MET:HA    | 2.47                     | 0.45              |
| 50:2p:148:LYS:CB   | 50:2p:150:MET:HE1  | 2.18                     | 0.45              |
| 55:2u:20:VAL:HA    | 55:2u:69:TRP:O     | 2.16                     | 0.45              |
| 56:2v:33:LEU:CD1   | 56:2v:34:PRO:HD2   | 2.34                     | 0.45              |
| 57:2w:108:LYS:H    | 57:2w:111:MET:CE   | 2.29                     | 0.45              |
| 61:20:39:LEU:O     | 61:20:40:ALA:HB3   | 2.17                     | 0.45              |
| 63:3A:51:LYS:HZ2   | 63:3A:76:ASP:HB3   | 1.82                     | 0.45              |
| 65:3C:43:ASN:OD1   | 65:3C:44:ILE:N     | 2.49                     | 0.45              |
| 68:3F:234:ASP:H    | 68:3F:252:THR:HB   | 1.81                     | 0.45              |
| 69:3G:114:LYS:HD2  | 69:3G:121:ARG:CZ   | 2.47                     | 0.45              |
| 69:3G:114:LYS:HG2  | 69:3G:121:ARG:HG3  | 1.98                     | 0.45              |
| 70:3H:14:LYS:NZ    | 70:3H:16:ILE:HB    | 2.32                     | 0.45              |
| 70:3H:233:ARG:NH1  | 70:3H:234:LEU:HD11 | 2.32                     | 0.45              |
| 73:3K:98:VAL:HG11  | 73:3K:115:LEU:HB2  | 1.97                     | 0.45              |
| 79:3Q:8:ARG:HG2    | 79:3Q:8:ARG:HH11   | 1.81                     | 0.45              |
| 1:1A:82:U:H2'      | 1:1A:83:C:O4'      | 2.17                     | 0.45              |
| 1:1A:223:G:N7      | 6:1F:165:LYS:HE3   | 2.32                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:248:C:O2'     | 1:1A:249:C:H5'     | 2.17                     | 0.45              |
| 1:1A:982:U:H2'     | 1:1A:983:C:H6      | 1.82                     | 0.45              |
| 1:1A:1586:G:HO2'   | 1:1A:1587:G:H5'    | 1.81                     | 0.45              |
| 1:1A:1596:U:O2'    | 18:2J:135:ARG:NH2  | 2.39                     | 0.45              |
| 1:1A:2607:C:H5''   | 20:2L:96:MET:HE1   | 1.99                     | 0.45              |
| 1:1A:2823:G:OP2    | 20:2L:20:LYS:HG3   | 2.17                     | 0.45              |
| 1:1A:3723:A:O2'    | 1:1A:3724:A:H5'    | 2.17                     | 0.45              |
| 1:1A:3856:A:H2'    | 1:1A:3857:G:H8     | 1.81                     | 0.45              |
| 1:1A:4249:G:H1'    | 13:2E:100:SER:OG   | 2.17                     | 0.45              |
| 7:1G:260:GLU:O     | 7:1G:260:GLU:HG2   | 2.17                     | 0.45              |
| 8:1H:106:VAL:O     | 8:1H:106:VAL:HG22  | 2.17                     | 0.45              |
| 8:1H:165:LEU:HD13  | 8:1H:176:THR:HG22  | 1.98                     | 0.45              |
| 11:2C:92:MET:HE1   | 11:2C:161:ILE:HG12 | 1.98                     | 0.45              |
| 11:2C:174:LYS:CG   | 11:2C:175:PHE:H    | 2.30                     | 0.45              |
| 15:2G:11:ARG:NH2   | 15:2G:61:ILE:HD11  | 2.32                     | 0.45              |
| 15:2G:103:LYS:CG   | 15:2G:103:LYS:O    | 2.64                     | 0.45              |
| 26:2R:115:LYS:HE2  | 26:2R:115:LYS:HB2  | 1.56                     | 0.45              |
| 46:2L:32:VAL:HG22  | 46:2L:33:GLU:N     | 2.30                     | 0.45              |
| 46:2L:54:ARG:HE    | 46:2L:152:LYS:CE   | 2.28                     | 0.45              |
| 47:2m:161:U:O2'    | 70:3H:87:ARG:NE    | 2.44                     | 0.45              |
| 47:2m:579:C:O2'    | 47:2m:580:U:P      | 2.75                     | 0.45              |
| 47:2m:614:C:H5''   | 47:2m:615:C:C6     | 2.52                     | 0.45              |
| 47:2m:841:G:OP2    | 76:3N:14:THR:HG22  | 2.16                     | 0.45              |
| 47:2m:845:G:C2'    | 47:2m:846:G:H5'    | 2.47                     | 0.45              |
| 47:2m:1008:A:O2'   | 47:2m:1009:A:H5'   | 2.17                     | 0.45              |
| 47:2m:1017:U:H2'   | 47:2m:1018:U:C6    | 2.52                     | 0.45              |
| 47:2m:1051:G:O2'   | 47:2m:1052:A:H5'   | 2.16                     | 0.45              |
| 47:2m:1302:G:O6    | 47:2m:1307:U:H5    | 2.00                     | 0.45              |
| 47:2m:1328:G:O2'   | 47:2m:1329:U:H5'   | 2.17                     | 0.45              |
| 47:2m:1547:C:N3    | 47:2m:1656:G:H1'   | 2.32                     | 0.45              |
| 47:2m:1627:C:H2'   | 47:2m:1628:C:C6    | 2.52                     | 0.45              |
| 47:2m:1731:A:H2'   | 47:2m:1732:G:H8    | 1.81                     | 0.45              |
| 48:2n:8:LEU:HA     | 48:2n:191:ARG:HH22 | 1.82                     | 0.45              |
| 50:2p:33:GLY:CA    | 50:2p:53:THR:HG23  | 2.44                     | 0.45              |
| 50:2p:59:LEU:CD2   | 50:2p:66:ILE:HD12  | 2.46                     | 0.45              |
| 52:2r:27:ASP:OD1   | 52:2r:27:ASP:N     | 2.49                     | 0.45              |
| 52:2r:125:SER:HB3  | 52:2r:203:ASN:ND2  | 2.29                     | 0.45              |
| 53:2s:45:ILE:HA    | 53:2s:64:VAL:HG13  | 1.99                     | 0.45              |
| 58:2x:42:ILE:HG23  | 58:2x:43:GLU:N     | 2.32                     | 0.45              |
| 59:2y:77:GLU:OE1   | 59:2y:77:GLU:N     | 2.50                     | 0.45              |
| 61:20:104:LEU:HD13 | 61:20:121:ARG:HH11 | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:3F:11:LEU:HD12  | 68:3F:307:VAL:HG12 | 1.99                     | 0.45              |
| 68:3F:174:VAL:HG23 | 68:3F:195:LEU:CD1  | 2.47                     | 0.45              |
| 68:3F:199:THR:HG22 | 68:3F:241:PHE:CD2  | 2.52                     | 0.45              |
| 68:3F:236:ILE:HD12 | 68:3F:237:ASN:N    | 2.32                     | 0.45              |
| 70:3H:230:LYS:O    | 70:3H:234:LEU:HB2  | 2.17                     | 0.45              |
| 71:3I:59:GLU:OE1   | 71:3I:59:GLU:CA    | 2.65                     | 0.45              |
| 73:3K:101:HIS:HD2  | 73:3K:102:LEU:HD22 | 1.81                     | 0.45              |
| 74:3L:64:ALA:O     | 74:3L:65:ASP:HB3   | 2.17                     | 0.45              |
| 1:1A:1:C:O2'       | 1:1A:2:G:P         | 2.74                     | 0.45              |
| 1:1A:182:G:H2'     | 1:1A:183:C:H4'     | 1.99                     | 0.45              |
| 1:1A:216:C:C6      | 1:1A:217:C:H5''    | 2.50                     | 0.45              |
| 1:1A:485:C:H2'     | 1:1A:486:C:OP1     | 2.17                     | 0.45              |
| 1:1A:1632:A:N3     | 1:1A:1632:A:H2'    | 2.32                     | 0.45              |
| 1:1A:1783:C:HO2'   | 1:1A:1784:U:H5'    | 1.82                     | 0.45              |
| 1:1A:2033:A:N3     | 1:1A:2034:G:C8     | 2.85                     | 0.45              |
| 1:1A:2079:G:H2'    | 1:1A:2080:U:H6     | 1.79                     | 0.45              |
| 1:1A:2293:U:H2'    | 1:1A:2294:G:H8     | 1.82                     | 0.45              |
| 1:1A:3781:C:O2'    | 1:1A:3782:C:H5'    | 2.16                     | 0.45              |
| 1:1A:3934:G:H2'    | 1:1A:3935:C:H6     | 1.81                     | 0.45              |
| 1:1A:3971:G:C6     | 1:1A:4049:U:H5'    | 2.51                     | 0.45              |
| 1:1A:4104:G:O2'    | 1:1A:4105:A:H5'    | 2.16                     | 0.45              |
| 1:1A:4290:U:OP1    | 43:2i:9[B]:ARG:HD2 | 2.16                     | 0.45              |
| 1:1A:4516:G:O2'    | 1:1A:4517:A:H5'    | 2.17                     | 0.45              |
| 1:1A:4648:A:O2'    | 1:1A:4649:G:H5'    | 2.17                     | 0.45              |
| 5:1E:45:ALA:HB3    | 5:1E:183:ILE:HG23  | 1.99                     | 0.45              |
| 7:1G:211:LEU:HD12  | 7:1G:223:PHE:HE2   | 1.82                     | 0.45              |
| 8:1H:198:SER:OG    | 8:1H:288:PHE:OXT   | 2.26                     | 0.45              |
| 14:2F:79:GLU:OE1   | 14:2F:79:GLU:N     | 2.49                     | 0.45              |
| 15:2G:126:GLU:OE1  | 15:2G:126:GLU:C    | 2.60                     | 0.45              |
| 18:2J:3:ARG:HD3    | 18:2J:3:ARG:HA     | 1.80                     | 0.45              |
| 18:2J:4:TYR:CE2    | 18:2J:16:LYS:HB2   | 2.52                     | 0.45              |
| 20:2L:44:LEU:HD22  | 20:2L:49:LEU:HD22  | 1.97                     | 0.45              |
| 23:2O:36:ALA:O     | 23:2O:40:GLU:CG    | 2.60                     | 0.45              |
| 23:2O:75:GLU:OE1   | 23:2O:75:GLU:N     | 2.50                     | 0.45              |
| 27:2S:101:PRO:O    | 27:2S:104:VAL:HG22 | 2.16                     | 0.45              |
| 33:2Y:81:ASN:OD1   | 33:2Y:84:GLU:HB2   | 2.17                     | 0.45              |
| 39:2e:29:LYS:HE3   | 39:2e:29:LYS:HB2   | 1.61                     | 0.45              |
| 41:2g:99:CYS:HB3   | 41:2g:115:CYS:HB3  | 1.98                     | 0.45              |
| 43:2i:14:LYS:HE3   | 43:2i:77:CYS:O     | 2.17                     | 0.45              |
| 47:2m:37:C:H2'     | 47:2m:38:A:O4'     | 2.17                     | 0.45              |
| 47:2m:203:G:H2'    | 47:2m:204:G:H8     | 1.82                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:874:G:H2'   | 47:2m:875:A:C8     | 2.51                     | 0.45              |
| 47:2m:1109:C:O2'  | 47:2m:1110:G:C5'   | 2.65                     | 0.45              |
| 47:2m:1156:U:O4   | 69:3G:194:ARG:NH1  | 2.49                     | 0.45              |
| 47:2m:1312:G:O6   | 72:3J:36:ARG:HG2   | 2.16                     | 0.45              |
| 60:2z:23:ARG:CG   | 77:3O:48:VAL:HG11  | 2.46                     | 0.45              |
| 61:20:16:ARG:HG3  | 61:20:16:ARG:HH11  | 1.80                     | 0.45              |
| 63:3A:52:THR:HG21 | 69:3G:261:PHE:HB3  | 1.99                     | 0.45              |
| 65:3C:42:ARG:HG2  | 65:3C:42:ARG:HH11  | 1.82                     | 0.45              |
| 68:3F:258:ILE:O   | 68:3F:267:VAL:HG23 | 2.16                     | 0.45              |
| 69:3G:60:TRP:CZ2  | 69:3G:62:PRO:HB3   | 2.51                     | 0.45              |
| 70:3H:32:MET:SD   | 70:3H:54:GLY:HA2   | 2.57                     | 0.45              |
| 74:3L:99:ALA:N    | 74:3L:133:THR:HG23 | 2.30                     | 0.45              |
| 77:3O:101:SER:C   | 77:3O:102:LYS:HD3  | 2.42                     | 0.45              |
| 1:1A:153:G:H2'    | 1:1A:154:G:H8      | 1.82                     | 0.45              |
| 1:1A:231:U:O2'    | 27:2S:103:LYS:HE2  | 2.17                     | 0.45              |
| 1:1A:323:C:H2'    | 1:1A:324:A:H8      | 1.82                     | 0.45              |
| 1:1A:426:A:H2'    | 1:1A:427:A:H8      | 1.82                     | 0.45              |
| 1:1A:909:A:H2'    | 1:1A:910:G:C8      | 2.52                     | 0.45              |
| 1:1A:1316:G:OP1   | 33:2Y:40:GLY:HA3   | 2.17                     | 0.45              |
| 1:1A:1327:C:H2'   | 1:1A:1328:G:H8     | 1.80                     | 0.45              |
| 1:1A:1504:G:H2'   | 1:1A:1505:C:H6     | 1.82                     | 0.45              |
| 1:1A:1791:U:C2'   | 1:1A:1792:U:H5'    | 2.42                     | 0.45              |
| 1:1A:1881:C:H5'   | 1:1A:2281:U:H1'    | 1.99                     | 0.45              |
| 1:1A:2257:C:N4    | 1:1A:2261:G:H1     | 2.15                     | 0.45              |
| 1:1A:2386:U:H2'   | 1:1A:2387:G:C8     | 2.51                     | 0.45              |
| 1:1A:2639:U:O2'   | 1:1A:2640:G:O5'    | 2.34                     | 0.45              |
| 1:1A:2683:C:H2'   | 1:1A:2684:C:H6     | 1.81                     | 0.45              |
| 1:1A:3868:G:N2    | 1:1A:3900:G:H1'    | 2.31                     | 0.45              |
| 1:1A:3965:A:C2    | 1:1A:4039:G:H5''   | 2.51                     | 0.45              |
| 1:1A:4257:A:C2    | 13:2E:27:GLY:HA2   | 2.52                     | 0.45              |
| 1:1A:4384:U:O3'   | 1:1A:4385:A:H3'    | 2.16                     | 0.45              |
| 1:1A:4475:G:N7    | 41:2g:125:LYS:HE2  | 2.31                     | 0.45              |
| 1:1A:4919:G:H2'   | 1:1A:4920:C:O4'    | 2.17                     | 0.45              |
| 1:1A:5023:C:H2'   | 1:1A:5024:C:O3'    | 2.17                     | 0.45              |
| 4:1D:113:VAL:HB   | 4:1D:164:ALA:HB1   | 1.99                     | 0.45              |
| 9:2A:52:GLU:HG3   | 30:2V:96:LEU:HD11  | 1.95                     | 0.45              |
| 12:2D:19:LYS:CB   | 12:2D:26:VAL:HG11  | 2.47                     | 0.45              |
| 17:2I:81:TRP:CZ2  | 17:2I:99:LEU:HD21  | 2.52                     | 0.45              |
| 23:2O:70:ILE:HD12 | 23:2O:70:ILE:N     | 2.31                     | 0.45              |
| 27:2S:67:ILE:HD12 | 27:2S:107:THR:HG21 | 1.99                     | 0.45              |
| 37:2c:58:MET:HE2  | 37:2c:90:LEU:CD2   | 2.41                     | 0.45              |

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| Atom-1               | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-----------------------|--------------------------|-------------------|
| 47:2m:418:A:H2'      | 47:2m:419:G:O5'       | 2.17                     | 0.45              |
| 47:2m:943:U:H2'      | 47:2m:944:A:H8        | 1.83                     | 0.45              |
| 47:2m:1531:A:H2'     | 47:2m:1532:C:C6       | 2.52                     | 0.45              |
| 47:2m:1688:C:H2'     | 47:2m:1689:C:C6       | 2.52                     | 0.45              |
| 47:2m:1693:G:H21     | 47:2m:1834:A:H8       | 1.64                     | 0.45              |
| 48:2n:52:LYS:HZ3     | 63:3A:83:PHE:HA       | 1.82                     | 0.45              |
| 51:2q:156:VAL:O      | 51:2q:157:ASN:HB2     | 2.16                     | 0.45              |
| 58:2x:92:LEU:CD1     | 58:2x:108:ILE:HD12    | 2.47                     | 0.45              |
| 58:2x:105:LYS:HE2    | 58:2x:109:LYS:HD2     | 1.97                     | 0.45              |
| 58:2x:116:ASP:OD1    | 58:2x:118:THR:HG22    | 2.17                     | 0.45              |
| 62:21:51:LYS:HG2     | 62:21:90:ASP:HB2      | 1.98                     | 0.45              |
| 63:3A:23:ILE:HD11    | 69:3G:251:LEU:HD13    | 1.98                     | 0.45              |
| 64:3B:48:LYS:HD3     | 64:3B:99:GLU:OE2      | 2.17                     | 0.45              |
| 65:3C:26:CYS:SG      | 65:3C:28:ARG:HB3      | 2.57                     | 0.45              |
| 68:3F:32:LEU:HD13    | 68:3F:40:ILE:CG2      | 2.47                     | 0.45              |
| 68:3F:59:LEU:HB3     | 68:3F:90:TRP:CZ3      | 2.52                     | 0.45              |
| 71:3I:138[B]:ARG:HB2 | 71:3I:139:LYS:HD3     | 1.99                     | 0.45              |
| 75:3M:28:ARG:HB3     | 75:3M:29:PRO:CD       | 2.37                     | 0.45              |
| 76:3N:110:ARG:HG2    | 76:3N:113[B]:ARG:HH21 | 1.81                     | 0.45              |
| 80:3R:140:TYR:CE1    | 80:3R:145:CYS:HA      | 2.51                     | 0.45              |
| 1:1A:180:C:H2'       | 1:1A:181:C:O4'        | 2.17                     | 0.44              |
| 1:1A:256:G:C2'       | 1:1A:257:C:H5'        | 2.47                     | 0.44              |
| 1:1A:666:G:H2'       | 1:1A:668:C:OP1        | 2.17                     | 0.44              |
| 1:1A:755:C:H2'       | 1:1A:756:G:C8         | 2.52                     | 0.44              |
| 1:1A:1100:U:H1'      | 1:1A:1167:C:N4        | 2.32                     | 0.44              |
| 1:1A:1356:U:H2'      | 1:1A:1357:C:C6        | 2.52                     | 0.44              |
| 1:1A:1433:A:H3'      | 1:1A:1434:G:H8        | 1.82                     | 0.44              |
| 1:1A:1557:C:H2'      | 1:1A:1558:A:H8        | 1.82                     | 0.44              |
| 1:1A:1908:A:H2'      | 1:1A:1909:G:O4'       | 2.17                     | 0.44              |
| 1:1A:2055:G:H3'      | 1:1A:2056:G:H5'       | 1.97                     | 0.44              |
| 1:1A:2389:A:O2'      | 1:1A:2390:G:P         | 2.74                     | 0.44              |
| 1:1A:2846:G:H21      | 24:2P:21:PRO:HG3      | 1.81                     | 0.44              |
| 1:1A:3610:A:H2'      | 1:1A:3611:A:C8        | 2.52                     | 0.44              |
| 1:1A:3668:C:OP1      | 4:1D:8:GLN:HG2        | 2.16                     | 0.44              |
| 1:1A:3778:U:O2       | 1:1A:3778:U:H2'       | 2.16                     | 0.44              |
| 1:1A:3944:G:H2'      | 1:1A:3945:A:H8        | 1.82                     | 0.44              |
| 1:1A:4110:C:H3'      | 1:1A:4111:U:C5        | 2.52                     | 0.44              |
| 1:1A:4178:A:C2       | 1:1A:4179:G:C5        | 3.05                     | 0.44              |
| 1:1A:4903:G:C2'      | 1:1A:4904:G:H5'       | 2.47                     | 0.44              |
| 1:1A:4934:A:H2'      | 1:1A:4935:C:H6        | 1.80                     | 0.44              |
| 4:1D:245:ARG:HA      | 4:1D:245:ARG:HD2      | 1.74                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:77:THR:HG21   | 5:1E:337:VAL:HG22  | 1.97                     | 0.44              |
| 5:1E:354:GLN:O     | 5:1E:360:LEU:HD11  | 2.17                     | 0.44              |
| 6:1F:163:LYS:HB2   | 6:1F:166:GLU:HG2   | 1.99                     | 0.44              |
| 8:1H:170:SER:OG    | 8:1H:214:ASP:OD2   | 2.11                     | 0.44              |
| 8:1H:203:ILE:HD13  | 8:1H:203:ILE:N     | 2.31                     | 0.44              |
| 9:2A:112:LEU:O     | 9:2A:113:ARG:HB2   | 2.18                     | 0.44              |
| 9:2A:114:LEU:HD22  | 9:2A:119:ASN:O     | 2.17                     | 0.44              |
| 10:2B:115:LEU:HD12 | 10:2B:115:LEU:C    | 2.42                     | 0.44              |
| 11:2C:53:LYS:HA    | 11:2C:53:LYS:HE3   | 1.99                     | 0.44              |
| 12:2D:99:ILE:HG22  | 12:2D:123:GLN:HB3  | 1.99                     | 0.44              |
| 13:2E:35:ARG:O     | 13:2E:39:VAL:HG12  | 2.17                     | 0.44              |
| 18:2J:153:LYS:HA   | 18:2J:153:LYS:HD3  | 1.69                     | 0.44              |
| 24:2P:48:ARG:NH1   | 24:2P:49:LEU:HB3   | 2.32                     | 0.44              |
| 25:2Q:121:ALA:HA   | 25:2Q:124:LYS:HG2  | 1.98                     | 0.44              |
| 46:2L:30:GLU:HG2   | 46:2L:208:SER:OG   | 2.17                     | 0.44              |
| 47:2m:964:A:H2'    | 47:2m:965:U:C6     | 2.52                     | 0.44              |
| 47:2m:988:C:H5''   | 49:2o:116:LYS:CG   | 2.46                     | 0.44              |
| 47:2m:1262:C:H5''  | 47:2m:1263:U:C6    | 2.51                     | 0.44              |
| 47:2m:1446:A:H5''  | 62:21:58:THR:HG23  | 1.98                     | 0.44              |
| 47:2m:1558:C:H2'   | 47:2m:1559:C:H6    | 1.78                     | 0.44              |
| 47:2m:1668:U:H6    | 47:2m:1668:U:O5'   | 2.00                     | 0.44              |
| 48:2n:6:ASP:O      | 48:2n:9:GLN:HG2    | 2.17                     | 0.44              |
| 50:2p:141:LYS:HZ1  | 50:2p:179:GLN:HG2  | 1.82                     | 0.44              |
| 52:2r:33:ILE:HA    | 52:2r:36:GLN:CG    | 2.47                     | 0.44              |
| 57:2w:127:LYS:HZ1  | 57:2w:128:HIS:HB3  | 1.80                     | 0.44              |
| 59:2y:34:VAL:O     | 59:2y:37:GLU:HG3   | 2.17                     | 0.44              |
| 62:21:104:ILE:HG23 | 62:21:105:SER:N    | 2.32                     | 0.44              |
| 69:3G:262:THR:HG22 | 69:3G:263:LYS:N    | 2.32                     | 0.44              |
| 70:3H:120:ASP:O    | 70:3H:121:ILE:HD12 | 2.16                     | 0.44              |
| 71:3I:128:VAL:O    | 71:3I:132:GLN:CG   | 2.65                     | 0.44              |
| 75:3M:74:VAL:HG22  | 75:3M:75:ILE:N     | 2.33                     | 0.44              |
| 1:1A:742:G:H2'     | 1:1A:743:G:C8      | 2.48                     | 0.44              |
| 1:1A:1397:A:O2'    | 1:1A:1467:C:O2'    | 2.33                     | 0.44              |
| 1:1A:1705:G:H2'    | 1:1A:1706:A:O4'    | 2.18                     | 0.44              |
| 1:1A:2051:C:H2'    | 1:1A:2052:G:O4'    | 2.17                     | 0.44              |
| 1:1A:2413:U:H2'    | 1:1A:2414:G:C8     | 2.52                     | 0.44              |
| 1:1A:2692:U:C2'    | 1:1A:2693:G:H5'    | 2.48                     | 0.44              |
| 1:1A:2702:C:C2'    | 1:1A:2703:G:H5'    | 2.47                     | 0.44              |
| 1:1A:2889:G:H2'    | 1:1A:2890:C:C6     | 2.52                     | 0.44              |
| 1:1A:3764:U:O2'    | 1:1A:3766:A:N6     | 2.51                     | 0.44              |
| 1:1A:3821:A:O2'    | 1:1A:3822:U:H5'    | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4413:C:H2'    | 1:1A:4414:A:O4'    | 2.18                     | 0.44              |
| 3:1C:135:C:OP1     | 26:2R:63:LYS:HD2   | 2.18                     | 0.44              |
| 9:2A:92:VAL:O      | 9:2A:120:GLY:HA2   | 2.17                     | 0.44              |
| 13:2E:141:ILE:HD11 | 13:2E:151:ILE:HA   | 1.99                     | 0.44              |
| 17:2I:34:VAL:HG22  | 17:2I:103:LYS:HB2  | 1.99                     | 0.44              |
| 19:2K:35:LEU:O     | 19:2K:39:THR:HB    | 2.18                     | 0.44              |
| 21:2M:15:ARG:HB3   | 21:2M:27:LEU:CD2   | 2.47                     | 0.44              |
| 26:2R:153:ILE:CG2  | 26:2R:155:ILE:HG23 | 2.45                     | 0.44              |
| 47:2m:213:G:O2'    | 47:2m:214:U:P      | 2.73                     | 0.44              |
| 47:2m:433:A:O2'    | 47:2m:434:G:H5'    | 2.17                     | 0.44              |
| 47:2m:896:U:H2'    | 47:2m:897:U:C4     | 2.52                     | 0.44              |
| 47:2m:1005:G:H2'   | 47:2m:1006:C:C6    | 2.48                     | 0.44              |
| 47:2m:1298:G:O2'   | 47:2m:1299:A:O4'   | 2.35                     | 0.44              |
| 47:2m:1400:U:H5''  | 47:2m:1401:A:OP2   | 2.18                     | 0.44              |
| 47:2m:1532:C:OP1   | 47:2m:1604:G:O2'   | 2.34                     | 0.44              |
| 47:2m:1589:A:O3'   | 61:20:82:ARG:HG3   | 2.17                     | 0.44              |
| 47:2m:1685:U:C4    | 47:2m:1686:G:N7    | 2.86                     | 0.44              |
| 47:2m:1860:A:P     | 65:3C:8:ASN:HB3    | 2.57                     | 0.44              |
| 50:2p:70:THR:HG22  | 50:2p:86:LEU:CD1   | 2.47                     | 0.44              |
| 53:2s:58:LYS:HE3   | 53:2s:90:LYS:CD    | 2.47                     | 0.44              |
| 53:2s:147:LYS:HA   | 75:3M:49:GLU:CD    | 2.41                     | 0.44              |
| 54:2t:139:LYS:HE3  | 54:2t:139:LYS:HB3  | 1.68                     | 0.44              |
| 54:2t:172:LEU:CD1  | 54:2t:190:LEU:HD12 | 2.42                     | 0.44              |
| 55:2u:16:PHE:HE1   | 55:2u:80:ARG:HG3   | 1.82                     | 0.44              |
| 56:2v:102:PHE:O    | 64:3B:8:ARG:HA     | 2.17                     | 0.44              |
| 57:2w:18:ARG:HG2   | 57:2w:18:ARG:HH11  | 1.83                     | 0.44              |
| 58:2x:34:VAL:HG13  | 58:2x:70:VAL:CB    | 2.25                     | 0.44              |
| 58:2x:89:SER:HA    | 58:2x:92:LEU:HD23  | 1.99                     | 0.44              |
| 59:2y:17:ILE:HD11  | 59:2y:54:VAL:HG22  | 1.99                     | 0.44              |
| 60:2z:65:GLU:OE1   | 60:2z:65:GLU:HA    | 2.17                     | 0.44              |
| 60:2z:120:HIS:O    | 60:2z:124:ARG:HG3  | 2.16                     | 0.44              |
| 61:20:38:LYS:HD3   | 61:20:41:LYS:HA    | 1.99                     | 0.44              |
| 70:3H:38:ALA:CB    | 70:3H:41:LEU:HD21  | 2.46                     | 0.44              |
| 70:3H:39:ASP:HB3   | 70:3H:46:LYS:HZ2   | 1.82                     | 0.44              |
| 72:3J:48:HIS:CD2   | 72:3J:114:TYR:HE1  | 2.35                     | 0.44              |
| 72:3J:61:TYR:OH    | 72:3J:108:CYS:HB3  | 2.16                     | 0.44              |
| 72:3J:84:LYS:HD3   | 72:3J:88:TRP:CZ2   | 2.52                     | 0.44              |
| 1:1A:1:C:C4'       | 1:1A:2:G:O4'       | 2.65                     | 0.44              |
| 1:1A:478:G:OP1     | 45:2k:66:ARG:NH1   | 2.49                     | 0.44              |
| 1:1A:496:G:N2      | 1:1A:658:C:O2'     | 2.51                     | 0.44              |
| 1:1A:759:G:OP1     | 11:2C:50:LYS:NZ    | 2.43                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1411:C:O3'   | 1:1A:1412:G:H8     | 2.00                     | 0.44              |
| 1:1A:1987:C:H2'   | 1:1A:1989:G:N2     | 2.30                     | 0.44              |
| 1:1A:2374:A:H2'   | 1:1A:2375:A:H8     | 1.82                     | 0.44              |
| 1:1A:2732:G:O2'   | 1:1A:2733:C:H5'    | 2.17                     | 0.44              |
| 1:1A:2752:G:H2'   | 1:1A:2753:G:C8     | 2.52                     | 0.44              |
| 1:1A:3770:U:H2'   | 1:1A:3771:C:H5'    | 1.97                     | 0.44              |
| 1:1A:3962:A:O2'   | 1:1A:3963:A:OP2    | 2.32                     | 0.44              |
| 1:1A:3969:G:N2    | 1:1A:4052:C:H2'    | 2.32                     | 0.44              |
| 1:1A:4578:G:H2'   | 1:1A:4579:U:H6     | 1.81                     | 0.44              |
| 1:1A:4606:G:H2'   | 1:1A:4607:A:C8     | 2.52                     | 0.44              |
| 1:1A:4629:U:C2    | 1:1A:4630:G:C8     | 3.05                     | 0.44              |
| 1:1A:4761:G:H2'   | 1:1A:4762:A:O4'    | 2.16                     | 0.44              |
| 2:1B:42:A:H1'     | 13:2E:75:ARG:CZ    | 2.47                     | 0.44              |
| 7:1G:52:ILE:HA    | 7:1G:147:ASP:HB3   | 1.99                     | 0.44              |
| 9:2A:67:THR:O     | 9:2A:71:MET:HG2    | 2.15                     | 0.44              |
| 15:2G:52:PHE:HD1  | 15:2G:55:MET:HE2   | 1.83                     | 0.44              |
| 15:2G:71:LYS:HG3  | 15:2G:72:TYR:N     | 2.32                     | 0.44              |
| 17:2I:89:PRO:O    | 17:2I:95:GLY:HA3   | 2.18                     | 0.44              |
| 18:2J:13:LYS:HB3  | 18:2J:152:GLU:HB3  | 1.99                     | 0.44              |
| 23:2O:56:LEU:HD12 | 23:2O:56:LEU:N     | 2.33                     | 0.44              |
| 27:2S:56:GLN:CG   | 27:2S:105:VAL:HG13 | 2.47                     | 0.44              |
| 29:2U:63:LEU:CD1  | 29:2U:65:ARG:HG2   | 2.47                     | 0.44              |
| 35:2a:60:ARG:HB2  | 35:2a:63:VAL:HG12  | 1.98                     | 0.44              |
| 37:2c:19:LYS:HE2  | 37:2c:21:VAL:CG2   | 2.47                     | 0.44              |
| 37:2c:80:HIS:NE2  | 37:2c:84:LYS:HD3   | 2.32                     | 0.44              |
| 47:2m:216:C:H2'   | 47:2m:217:A:H5'    | 1.98                     | 0.44              |
| 47:2m:352:U:H2'   | 47:2m:353:C:H6     | 1.82                     | 0.44              |
| 47:2m:367:U:O2'   | 47:2m:371:A:N7     | 2.44                     | 0.44              |
| 47:2m:478:G:O2'   | 47:2m:479:C:H5'    | 2.17                     | 0.44              |
| 47:2m:837:A:H61   | 76:3N:9:THR:CB     | 2.31                     | 0.44              |
| 47:2m:1203:G:H2'  | 47:2m:1204:A:N3    | 2.32                     | 0.44              |
| 47:2m:1686:G:C2   | 47:2m:1687:C:C6    | 3.04                     | 0.44              |
| 47:2m:1739:C:H2'  | 47:2m:1740:C:H6    | 1.82                     | 0.44              |
| 49:2o:216:LYS:HB3 | 49:2o:216:LYS:HE2  | 1.76                     | 0.44              |
| 50:2p:189:MET:HB2 | 50:2p:189:MET:HE2  | 1.78                     | 0.44              |
| 52:2r:44:LYS:HD3  | 52:2r:44:LYS:C     | 2.41                     | 0.44              |
| 53:2s:142:LYS:HB3 | 53:2s:144:ILE:CD1  | 2.47                     | 0.44              |
| 54:2t:64:ASN:O    | 54:2t:186:ASP:HA   | 2.17                     | 0.44              |
| 58:2x:39:LEU:HB3  | 58:2x:51:LEU:HD21  | 1.99                     | 0.44              |
| 58:2x:101:ASP:OD1 | 58:2x:101:ASP:N    | 2.50                     | 0.44              |
| 65:3C:81:SER:O    | 65:3C:82:LYS:HB2   | 2.16                     | 0.44              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 66:3D:35:MET:O     | 66:3D:35:MET:HG3     | 2.18                     | 0.44              |
| 68:3F:59:LEU:HD21  | 68:3F:95:GLY:HA2     | 1.99                     | 0.44              |
| 68:3F:104:HIS:CD2  | 68:3F:124:SER:HB3    | 2.53                     | 0.44              |
| 69:3G:166:ARG:NH1  | 69:3G:255:LEU:HD11   | 2.32                     | 0.44              |
| 71:3I:137:VAL:HG12 | 71:3I:138[B]:ARG:HG3 | 1.98                     | 0.44              |
| 72:3J:74:ILE:HG22  | 72:3J:75:ASN:O       | 2.17                     | 0.44              |
| 76:3N:7:ILE:CG2    | 76:3N:25:ILE:HG23    | 2.48                     | 0.44              |
| 80:3R:140:TYR:CZ   | 80:3R:145:CYS:HA     | 2.52                     | 0.44              |
| 1:1A:100:C:H2'     | 1:1A:101:A:O4'       | 2.17                     | 0.44              |
| 1:1A:216:C:O3'     | 1:1A:219:G:N2        | 2.51                     | 0.44              |
| 1:1A:507:G:O2'     | 1:1A:508:G:H5'       | 2.17                     | 0.44              |
| 1:1A:1194:G:H2'    | 1:1A:1195:G:C8       | 2.53                     | 0.44              |
| 1:1A:1794:A:H5''   | 1:1A:4214:A:N6       | 2.32                     | 0.44              |
| 1:1A:1835:G:H4'    | 1:1A:1836:G:H5''     | 1.98                     | 0.44              |
| 1:1A:1867:A:H2'    | 1:1A:1868:A:C8       | 2.52                     | 0.44              |
| 1:1A:2098:G:HO2'   | 1:1A:2099:G:P        | 2.34                     | 0.44              |
| 1:1A:2843:U:H5''   | 81:1A:5104:84D:C5    | 2.47                     | 0.44              |
| 1:1A:3910:C:C2     | 1:1A:3911:C:C5       | 3.05                     | 0.44              |
| 1:1A:4125:C:O2'    | 1:1A:4126:C:H5'      | 2.18                     | 0.44              |
| 1:1A:4415:A:C2     | 1:1A:4428:A:H1'      | 2.51                     | 0.44              |
| 1:1A:4440:G:O2'    | 12:2D:103:LEU:HB3    | 2.17                     | 0.44              |
| 1:1A:4876:U:H2'    | 21:2M:169:THR:HB     | 2.00                     | 0.44              |
| 1:1A:4888:U:O4     | 1:1A:4933:C:O2       | 2.35                     | 0.44              |
| 3:1C:19:C:C2       | 3:1C:20:A:C8         | 3.06                     | 0.44              |
| 6:1F:154:VAL:HG22  | 6:1F:155:GLU:H       | 1.81                     | 0.44              |
| 7:1G:117:LYS:N     | 7:1G:117:LYS:HD2     | 2.32                     | 0.44              |
| 8:1H:162:VAL:HG21  | 8:1H:175:VAL:CG1     | 2.48                     | 0.44              |
| 10:2B:70:LEU:HD23  | 10:2B:70:LEU:HA      | 1.87                     | 0.44              |
| 12:2D:91:LEU:HD11  | 12:2D:129:VAL:HG11   | 2.00                     | 0.44              |
| 13:2E:117:ILE:HG22 | 13:2E:118:LYS:N      | 2.33                     | 0.44              |
| 13:2E:175:LEU:HD12 | 13:2E:176:PRO:HD2    | 1.99                     | 0.44              |
| 20:2L:163:ARG:HD2  | 47:2m:871:U:O2       | 2.18                     | 0.44              |
| 31:2W:57:LYS:O     | 31:2W:61:GLU:HG3     | 2.17                     | 0.44              |
| 43:2i:20:PRO:HB2   | 43:2i:73:VAL:CG2     | 2.48                     | 0.44              |
| 47:2m:70:G:N2      | 47:2m:80:G:C6        | 2.85                     | 0.44              |
| 47:2m:148:U:HO2'   | 47:2m:149:A:P        | 2.38                     | 0.44              |
| 47:2m:150:A:N3     | 47:2m:150:A:H2'      | 2.32                     | 0.44              |
| 47:2m:216:C:O2     | 47:2m:216:C:O4'      | 2.35                     | 0.44              |
| 47:2m:355:G:OP1    | 56:2v:92:TYR:OH      | 2.31                     | 0.44              |
| 47:2m:481:C:H2'    | 47:2m:482:G:O4'      | 2.17                     | 0.44              |
| 47:2m:630:U:H3'    | 47:2m:630:U:O2       | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:810:A:C3'    | 47:2m:811:A:H5'    | 2.47                     | 0.44              |
| 47:2m:1533:A:C8    | 47:2m:1604:G:H1'   | 2.53                     | 0.44              |
| 47:2m:1535:U:H2'   | 47:2m:1536:G:OP1   | 2.17                     | 0.44              |
| 47:2m:1578:U:H1'   | 50:2p:6:SER:OG     | 2.17                     | 0.44              |
| 47:2m:1610:G:C6    | 47:2m:1611:G:C6    | 3.06                     | 0.44              |
| 47:2m:1727:G:N7    | 81:2m:1901:84D:N2  | 2.66                     | 0.44              |
| 47:2m:1814:G:O3'   | 47:2m:1815:A:H8    | 2.00                     | 0.44              |
| 48:2n:3:GLY:HA3    | 48:2n:8:LEU:HD11   | 1.99                     | 0.44              |
| 48:2n:28:THR:HA    | 48:2n:45:GLY:O     | 2.17                     | 0.44              |
| 51:2q:97:GLU:HG2   | 51:2q:99:PHE:CZ    | 2.53                     | 0.44              |
| 51:2q:200:ARG:HG2  | 51:2q:206:ASP:OD2  | 2.17                     | 0.44              |
| 54:2t:191:GLU:HG3  | 56:2v:19:ASN:ND2   | 2.31                     | 0.44              |
| 57:2w:54:HIS:HA    | 57:2w:57:LEU:HD13  | 2.00                     | 0.44              |
| 63:3A:24:ILE:HD13  | 63:3A:31:SER:HB2   | 1.99                     | 0.44              |
| 68:3F:265:ILE:HD12 | 68:3F:265:ILE:HA   | 1.82                     | 0.44              |
| 69:3G:183:LYS:CD   | 69:3G:196:ILE:HG23 | 2.47                     | 0.44              |
| 70:3H:218:LYS:HE3  | 70:3H:219:GLU:N    | 2.32                     | 0.44              |
| 71:3I:102:ILE:HD12 | 71:3I:103:GLU:H    | 1.83                     | 0.44              |
| 73:3K:57:SER:OG    | 78:3P:54:VAL:HG13  | 2.18                     | 0.44              |
| 1:1A:343:C:C2'     | 1:1A:344:A:H5'     | 2.47                     | 0.44              |
| 1:1A:408:A:H5''    | 1:1A:409:G:P       | 2.57                     | 0.44              |
| 1:1A:504:G:C4'     | 1:1A:505:G:OP1     | 2.66                     | 0.44              |
| 1:1A:750:U:C2      | 1:1A:751:G:C8      | 3.05                     | 0.44              |
| 1:1A:1423:U:C2'    | 1:1A:1424:G:H5'    | 2.48                     | 0.44              |
| 1:1A:2017:A:H3'    | 1:1A:2018:C:H5     | 1.83                     | 0.44              |
| 1:1A:2431:A:H2'    | 1:1A:2432:U:C6     | 2.53                     | 0.44              |
| 1:1A:3599:A:O2'    | 1:1A:3600:G:H5'    | 2.18                     | 0.44              |
| 1:1A:3667:C:O2'    | 4:1D:11:GLY:HA3    | 2.18                     | 0.44              |
| 1:1A:3726:A:C2'    | 1:1A:3727:A:O5'    | 2.66                     | 0.44              |
| 1:1A:3890:A:C2'    | 1:1A:3891:A:H5'    | 2.47                     | 0.44              |
| 1:1A:4052:C:H6     | 1:1A:4052:C:P      | 2.41                     | 0.44              |
| 1:1A:4142:C:H5'    | 1:1A:4143:G:P      | 2.57                     | 0.44              |
| 1:1A:4766:C:O2'    | 1:1A:4767:C:H5'    | 2.17                     | 0.44              |
| 3:1C:40:A:H2'      | 3:1C:41:A:H8       | 1.83                     | 0.44              |
| 3:1C:81:C:O3'      | 3:1C:87:G:H5'      | 2.17                     | 0.44              |
| 4:1D:66:PRO:HG2    | 4:1D:67:TYR:CE2    | 2.53                     | 0.44              |
| 7:1G:41:LYS:HE3    | 22:2N:32:ARG:O     | 2.18                     | 0.44              |
| 9:2A:108:VAL:HG21  | 9:2A:135:ILE:HG21  | 1.98                     | 0.44              |
| 11:2C:107:GLU:O    | 11:2C:107:GLU:HG2  | 2.16                     | 0.44              |
| 14:2F:194:ILE:HD12 | 14:2F:194:ILE:HA   | 1.84                     | 0.44              |
| 15:2G:97:ALA:HB1   | 17:2I:200:GLY:O    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:2O:49:VAL:O    | 23:2O:49:VAL:HG23  | 2.17                     | 0.44              |
| 25:2Q:74:ARG:HE   | 47:2m:1748:G:H5'   | 1.80                     | 0.44              |
| 28:2T:103:ASP:HB3 | 28:2T:106:LEU:CD1  | 2.43                     | 0.44              |
| 29:2U:3:SER:HA    | 29:2U:6:ARG:HG3    | 2.00                     | 0.44              |
| 30:2V:65:MET:CA   | 30:2V:68:ARG:HH21  | 2.31                     | 0.44              |
| 47:2m:154:U:H5'   | 47:2m:155:G:OP2    | 2.17                     | 0.44              |
| 47:2m:574:A:H2'   | 47:2m:575:A:H8     | 1.83                     | 0.44              |
| 47:2m:1245:G:H2'  | 47:2m:1246:A:C8    | 2.52                     | 0.44              |
| 47:2m:1255:G:OP2  | 47:2m:1257:G:O2'   | 2.24                     | 0.44              |
| 47:2m:1454:A:H5'' | 59:2y:3:ARG:HD3    | 1.99                     | 0.44              |
| 47:2m:1650:A:C4   | 47:2m:1675:A:C6    | 3.06                     | 0.44              |
| 48:2n:51:LEU:HD23 | 59:2y:105:MET:HE1  | 1.98                     | 0.44              |
| 51:2q:200:ARG:HA  | 51:2q:206:ASP:OD1  | 2.18                     | 0.44              |
| 52:2r:179:ASN:HA  | 52:2r:182:LYS:HG2  | 1.99                     | 0.44              |
| 55:2u:52:LEU:CD2  | 55:2u:58:VAL:HG22  | 2.48                     | 0.44              |
| 56:2v:126:VAL:CG1 | 56:2v:128:VAL:HG13 | 2.47                     | 0.44              |
| 57:2w:56:LEU:O    | 57:2w:60:LEU:HD23  | 2.18                     | 0.44              |
| 58:2x:25:CYS:SG   | 58:2x:68:ILE:CD1   | 3.05                     | 0.44              |
| 58:2x:97:GLN:HG2  | 68:3F:60:ARG:NH2   | 2.33                     | 0.44              |
| 58:2x:106:LYS:HB3 | 58:2x:106:LYS:HE3  | 1.77                     | 0.44              |
| 59:2y:17:ILE:HA   | 59:2y:58:MET:HE1   | 2.00                     | 0.44              |
| 63:3A:62:MET:HG3  | 63:3A:64:GLU:H     | 1.83                     | 0.44              |
| 65:3C:46:GLU:O    | 65:3C:48:ALA:N     | 2.49                     | 0.44              |
| 68:3F:146:SER:HA  | 68:3F:177:TRP:CZ2  | 2.52                     | 0.44              |
| 68:3F:146:SER:OG  | 68:3F:147:HIS:N    | 2.50                     | 0.44              |
| 68:3F:173:LEU:HG  | 68:3F:189:ILE:CG2  | 2.38                     | 0.44              |
| 72:3J:67:ALA:HB2  | 80:3R:108:VAL:CG2  | 2.42                     | 0.44              |
| 1:1A:1241:C:H6    | 30:2V:118:LEU:HG   | 1.82                     | 0.44              |
| 1:1A:1751:A:H2'   | 1:1A:1752:G:C8     | 2.53                     | 0.44              |
| 1:1A:1879:C:C2'   | 1:1A:1880:G:H5'    | 2.48                     | 0.44              |
| 1:1A:1883:G:H5'   | 33:2Y:49:PHE:CE1   | 2.52                     | 0.44              |
| 1:1A:2634:C:O2'   | 1:1A:2635:U:H5'    | 2.17                     | 0.44              |
| 1:1A:2658:G:O6    | 31:2W:32:LYS:HE2   | 2.18                     | 0.44              |
| 1:1A:2767:U:H2'   | 1:1A:2769:U:C2     | 2.53                     | 0.44              |
| 1:1A:3653:A:C2    | 1:1A:3692:A:O4'    | 2.70                     | 0.44              |
| 1:1A:3933:G:O2'   | 1:1A:3934:G:H5'    | 2.18                     | 0.44              |
| 1:1A:4323:A:H4'   | 7:1G:176:SER:OG    | 2.18                     | 0.44              |
| 2:1B:33:U:HO2'    | 2:1B:34:C:P        | 2.41                     | 0.44              |
| 3:1C:37:A:H5''    | 3:1C:39:G:O4'      | 2.16                     | 0.44              |
| 11:2C:176:LEU:HB3 | 41:2g:86:ALA:HB1   | 1.98                     | 0.44              |
| 12:2D:180:GLU:HG3 | 12:2D:184:MET:SD   | 2.58                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:2S:72:GLN:HB3   | 27:2S:81:TYR:HB2   | 1.99                     | 0.44              |
| 32:2X:21:VAL:HG22  | 32:2X:22:THR:N     | 2.32                     | 0.44              |
| 32:2X:46:LEU:CD2   | 32:2X:72:VAL:HG11  | 2.46                     | 0.44              |
| 36:2b:35:LYS:HA    | 36:2b:44:LEU:HD21  | 1.98                     | 0.44              |
| 43:2i:33:LEU:O     | 43:2i:33:LEU:HG    | 2.18                     | 0.44              |
| 45:2k:20:ARG:HG3   | 45:2k:20:ARG:HH11  | 1.83                     | 0.44              |
| 47:2m:1:U:O2'      | 69:3G:205:VAL:HG22 | 2.18                     | 0.44              |
| 47:2m:50:A:C2'     | 47:2m:51:U:H5'     | 2.47                     | 0.44              |
| 47:2m:310:C:O2'    | 47:2m:311:C:H5'    | 2.17                     | 0.44              |
| 47:2m:332:G:O5'    | 70:3H:190:ARG:NH1  | 2.50                     | 0.44              |
| 47:2m:1127:C:H5''  | 78:3P:17:ARG:HH21  | 1.80                     | 0.44              |
| 47:2m:1302:G:N3    | 80:3R:95:ARG:NH1   | 2.65                     | 0.44              |
| 47:2m:1599:U:H4'   | 47:2m:1600:G:N3    | 2.32                     | 0.44              |
| 47:2m:1785:C:O2'   | 47:2m:1786:U:O5'   | 2.31                     | 0.44              |
| 48:2n:10:MET:HE3   | 59:2y:109:LEU:CD2  | 2.46                     | 0.44              |
| 49:2o:128:LYS:HE2  | 49:2o:129:THR:O    | 2.18                     | 0.44              |
| 49:2o:166:LYS:HB2  | 49:2o:166:LYS:HE3  | 1.67                     | 0.44              |
| 50:2p:42:THR:C     | 50:2p:44:THR:H     | 2.26                     | 0.44              |
| 51:2q:47:PHE:CD2   | 51:2q:90:ILE:HD12  | 2.52                     | 0.44              |
| 52:2r:128:ILE:HG22 | 52:2r:128:ILE:O    | 2.18                     | 0.44              |
| 54:2t:22:HIS:CD2   | 54:2t:22:HIS:C     | 2.96                     | 0.44              |
| 61:20:28:LEU:HD11  | 61:20:54:TYR:CE1   | 2.53                     | 0.44              |
| 64:3B:107:ARG:HD3  | 64:3B:112:VAL:HG22 | 2.00                     | 0.44              |
| 68:3F:163:PRO:O    | 68:3F:164:ILE:HG23 | 2.17                     | 0.44              |
| 69:3G:153:GLY:O    | 69:3G:156:ILE:HG12 | 2.18                     | 0.44              |
| 75:3M:55:ASP:OD2   | 75:3M:57:ARG:HG2   | 2.18                     | 0.44              |
| 76:3N:10:ARG:O     | 76:3N:24:VAL:HG23  | 2.18                     | 0.44              |
| 80:3R:137:ASP:O    | 80:3R:150:PHE:HB3  | 2.17                     | 0.44              |
| 1:1A:269:G:H2'     | 1:1A:270:U:H6      | 1.83                     | 0.44              |
| 1:1A:1535:C:H2'    | 1:1A:1536:U:O4'    | 2.17                     | 0.44              |
| 1:1A:2439:G:N3     | 1:1A:2439:G:H2'    | 2.32                     | 0.44              |
| 1:1A:2500:U:H2'    | 1:1A:2501:C:C6     | 2.53                     | 0.44              |
| 1:1A:2500:U:H2'    | 1:1A:2501:C:H6     | 1.83                     | 0.44              |
| 1:1A:2696:A:C5     | 39:2e:69:LEU:HD13  | 2.53                     | 0.44              |
| 1:1A:2751:G:C2     | 1:1A:2752:G:C8     | 3.05                     | 0.44              |
| 1:1A:3652:A:O2'    | 4:1D:182:ALA:HB2   | 2.18                     | 0.44              |
| 1:1A:4132:C:C2'    | 1:1A:4133:C:H5'    | 2.47                     | 0.44              |
| 1:1A:4305:G:H2'    | 1:1A:4305:G:N3     | 2.33                     | 0.44              |
| 1:1A:4320:G:H2'    | 1:1A:4321:U:O4'    | 2.17                     | 0.44              |
| 1:1A:4390:A:H2'    | 1:1A:4391:G:O4'    | 2.17                     | 0.44              |
| 1:1A:4434:C:O2'    | 1:1A:4435:U:H5'    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4435:U:H2'   | 1:1A:4436:U:C6     | 2.53                     | 0.44              |
| 1:1A:4750:G:H22   | 34:2Z:52:LYS:HE2   | 1.81                     | 0.44              |
| 2:1B:54:A:C5      | 13:2E:12:MET:HG3   | 2.53                     | 0.44              |
| 5:1E:66:LYS:HB3   | 24:2P:14:PHE:CE2   | 2.53                     | 0.44              |
| 6:1F:91:ALA:O     | 6:1F:92:PHE:HB2    | 2.17                     | 0.44              |
| 31:2W:20:LEU:HD23 | 31:2W:101:ASP:CB   | 2.34                     | 0.44              |
| 31:2W:52:CYS:SG   | 31:2W:53:PRO:HD2   | 2.58                     | 0.44              |
| 47:2m:600:G:H2'   | 47:2m:601:G:C8     | 2.52                     | 0.44              |
| 47:2m:604:A:O2'   | 47:2m:605:A:P      | 2.76                     | 0.44              |
| 47:2m:637:U:O2    | 79:3Q:56:ASN:ND2   | 2.51                     | 0.44              |
| 47:2m:846:G:OP2   | 51:2q:108:ARG:NH2  | 2.51                     | 0.44              |
| 47:2m:1258:A:H2'  | 47:2m:1259:A:OP1   | 2.17                     | 0.44              |
| 47:2m:1542:C:H5'' | 61:20:62:ARG:CZ    | 2.48                     | 0.44              |
| 47:2m:1606:G:H1'  | 47:2m:1633:A:H61   | 1.82                     | 0.44              |
| 47:2m:1641:A:C2'  | 47:2m:1642:U:H5'   | 2.48                     | 0.44              |
| 47:2m:1649:U:H5'  | 58:2x:128:GLU:HB2  | 2.00                     | 0.44              |
| 48:2n:136:GLU:HA  | 48:2n:139:TYR:HD2  | 1.82                     | 0.44              |
| 49:2o:30:TRP:CZ2  | 49:2o:48:LEU:HD23  | 2.52                     | 0.44              |
| 49:2o:42:ARG:NH2  | 49:2o:232:HIS:O    | 2.41                     | 0.44              |
| 49:2o:46:LYS:HE3  | 49:2o:46:LYS:HB3   | 1.74                     | 0.44              |
| 50:2p:169:ASP:OD1 | 50:2p:188:ILE:HB   | 2.17                     | 0.44              |
| 53:2s:95:ILE:HG22 | 53:2s:96:ALA:H     | 1.81                     | 0.44              |
| 54:2t:98:LYS:C    | 54:2t:98:LYS:HD3   | 2.43                     | 0.44              |
| 57:2w:49:LEU:O    | 57:2w:54:HIS:NE2   | 2.51                     | 0.44              |
| 60:2z:78:LYS:HD2  | 60:2z:78:LYS:C     | 2.35                     | 0.44              |
| 61:20:28:LEU:HB3  | 61:20:110:LEU:CD1  | 2.48                     | 0.44              |
| 66:3D:44:ARG:NH1  | 66:3D:44:ARG:HB3   | 2.33                     | 0.44              |
| 69:3G:135:GLY:CA  | 69:3G:165:VAL:HB   | 2.42                     | 0.44              |
| 70:3H:41:LEU:O    | 70:3H:41:LEU:HG    | 2.16                     | 0.44              |
| 74:3L:103:ASN:ND2 | 74:3L:140:THR:HG22 | 2.33                     | 0.44              |
| 75:3M:119:LYS:HB3 | 75:3M:121:THR:HG23 | 2.00                     | 0.44              |
| 77:3O:47:LEU:HD13 | 77:3O:79:ILE:CD1   | 2.47                     | 0.44              |
| 77:3O:73:VAL:HG22 | 77:3O:79:ILE:CG1   | 2.47                     | 0.44              |
| 1:1A:456:C:O2'    | 1:1A:457:G:P       | 2.76                     | 0.44              |
| 1:1A:498:C:N4     | 1:1A:656:C:H42     | 2.15                     | 0.44              |
| 1:1A:653:U:O2     | 1:1A:653:U:H2'     | 2.18                     | 0.44              |
| 1:1A:1275:G:O2'   | 1:1A:1276:C:O5'    | 2.25                     | 0.44              |
| 1:1A:1550:G:O2'   | 1:1A:1551:C:H5'    | 2.18                     | 0.44              |
| 1:1A:1564:A:H8    | 1:1A:1564:A:OP2    | 2.01                     | 0.44              |
| 1:1A:1855:G:OP1   | 30:2V:4:SER:HB2    | 2.17                     | 0.44              |
| 1:1A:2601:A:N6    | 1:1A:2744:A:OP2    | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2652:G:N2     | 44:2j:59:SER:O     | 2.50                     | 0.44              |
| 1:1A:2775:C:HO2'   | 1:1A:2776:G:P      | 2.41                     | 0.44              |
| 1:1A:2838:G:H2'    | 1:1A:2839:U:C6     | 2.53                     | 0.44              |
| 1:1A:3604:A:H2'    | 1:1A:3605:C:C5'    | 2.48                     | 0.44              |
| 1:1A:3888:G:O2'    | 1:1A:3889:G:P      | 2.75                     | 0.44              |
| 1:1A:4352:U:O2'    | 1:1A:4353:U:H5'    | 2.17                     | 0.44              |
| 1:1A:4358:U:H4'    | 14:2F:197:LYS:HD3  | 1.99                     | 0.44              |
| 1:1A:4767:C:O3'    | 1:1A:4874:A:N6     | 2.50                     | 0.44              |
| 2:1B:3:C:OP1       | 2:1B:58:A:H4'      | 2.18                     | 0.44              |
| 4:1D:14:SER:HA     | 4:1D:17:ARG:NE     | 2.24                     | 0.44              |
| 7:1G:256:LYS:NZ    | 7:1G:257:PRO:HD2   | 2.33                     | 0.44              |
| 10:2B:51:LEU:O     | 10:2B:55:VAL:HG13  | 2.18                     | 0.44              |
| 10:2B:140:VAL:HG21 | 10:2B:166:LEU:O    | 2.17                     | 0.44              |
| 11:2C:54:ARG:CZ    | 11:2C:54:ARG:HB2   | 2.48                     | 0.44              |
| 25:2Q:97:LYS:N     | 25:2Q:98:PRO:CD    | 2.81                     | 0.44              |
| 30:2V:65:MET:HG2   | 30:2V:68:ARG:NH2   | 2.33                     | 0.44              |
| 34:2Z:6:TRP:CE2    | 34:2Z:102:ARG:HD3  | 2.53                     | 0.44              |
| 34:2Z:48:ALA:HB2   | 34:2Z:71:TRP:CZ3   | 2.53                     | 0.44              |
| 46:2l:25:ARG:HD3   | 46:2l:210:MET:CE   | 2.47                     | 0.44              |
| 47:2m:5:U:OP2      | 69:3G:230:THR:OG1  | 2.35                     | 0.44              |
| 47:2m:321:C:H2'    | 47:2m:322:C:N1     | 2.32                     | 0.44              |
| 47:2m:392:A:C2'    | 47:2m:393:U:H5'    | 2.47                     | 0.44              |
| 47:2m:536:A:H5''   | 47:2m:537:C:O4'    | 2.16                     | 0.44              |
| 47:2m:856:C:O2'    | 47:2m:857:U:H5'    | 2.18                     | 0.44              |
| 47:2m:862:A:O2'    | 47:2m:863:U:H5'    | 2.17                     | 0.44              |
| 47:2m:1083:A:H4'   | 47:2m:1085:C:C4    | 2.52                     | 0.44              |
| 47:2m:1237:C:O3'   | 57:2w:129:GLY:HA3  | 2.17                     | 0.44              |
| 47:2m:1280:G:H2'   | 47:2m:1280:G:N3    | 2.33                     | 0.44              |
| 47:2m:1297:U:H1'   | 47:2m:1301:A:N1    | 2.33                     | 0.44              |
| 47:2m:1543:U:H4'   | 58:2x:43:GLU:HG2   | 1.98                     | 0.44              |
| 47:2m:1589:A:O3'   | 61:20:82:ARG:HD3   | 2.18                     | 0.44              |
| 48:2n:31:ASP:N     | 48:2n:150:THR:O    | 2.49                     | 0.44              |
| 50:2p:25:LEU:HD22  | 50:2p:69:LEU:HD11  | 1.98                     | 0.44              |
| 52:2r:201:LYS:HE3  | 52:2r:201:LYS:HB3  | 1.81                     | 0.44              |
| 53:2s:172:THR:O    | 53:2s:176:VAL:HG23 | 2.18                     | 0.44              |
| 54:2t:36:THR:O     | 54:2t:95:THR:HA    | 2.18                     | 0.44              |
| 57:2w:98:ASN:CA    | 57:2w:122:THR:HG22 | 2.48                     | 0.44              |
| 58:2x:60:LYS:HD3   | 58:2x:60:LYS:O     | 2.18                     | 0.44              |
| 60:2z:67:VAL:HA    | 60:2z:70:ILE:HG12  | 1.99                     | 0.44              |
| 63:3A:3:ASN:HB3    | 69:3G:169:TYR:OH   | 2.18                     | 0.44              |
| 64:3B:21:LYS:HD2   | 64:3B:27:TYR:CE2   | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:3C:82:LYS:HB2   | 65:3C:82:LYS:HE2   | 1.77                     | 0.44              |
| 65:3C:88:SER:O     | 65:3C:92:ARG:HG3   | 2.18                     | 0.44              |
| 66:3D:11:LEU:HD12  | 66:3D:55:VAL:HG21  | 1.98                     | 0.44              |
| 68:3F:92:LEU:O     | 68:3F:93:THR:OG1   | 2.30                     | 0.44              |
| 69:3G:60:TRP:CD1   | 69:3G:92:GLU:HG2   | 2.53                     | 0.44              |
| 69:3G:103:LYS:NZ   | 69:3G:132:ASP:HA   | 2.33                     | 0.44              |
| 70:3H:3:LEU:HD22   | 70:3H:111:LEU:HD12 | 2.00                     | 0.44              |
| 71:3I:25:LEU:HD22  | 71:3I:40:LYS:NZ    | 2.32                     | 0.44              |
| 1:1A:109:G:OP2     | 14:2F:74:ARG:NH2   | 2.49                     | 0.44              |
| 1:1A:422:C:H2'     | 1:1A:423:G:H8      | 1.82                     | 0.44              |
| 1:1A:731:G:C6      | 1:1A:932:A:C4      | 3.06                     | 0.44              |
| 1:1A:920:C:H2'     | 1:1A:921:C:C6      | 2.52                     | 0.44              |
| 1:1A:1298:C:H2'    | 1:1A:1299:G:H8     | 1.82                     | 0.44              |
| 1:1A:1420:A:H2'    | 1:1A:1420:A:N3     | 2.33                     | 0.44              |
| 1:1A:1734:G:N2     | 1:1A:1735:U:O4     | 2.34                     | 0.44              |
| 1:1A:1771:U:O2'    | 1:1A:1772:C:C6     | 2.71                     | 0.44              |
| 1:1A:2483:G:H2'    | 1:1A:2484:A:C4     | 2.53                     | 0.44              |
| 1:1A:2692:U:H2'    | 1:1A:2693:G:H5'    | 2.00                     | 0.44              |
| 1:1A:3757:G:O2'    | 1:1A:3758:U:H6     | 2.00                     | 0.44              |
| 1:1A:3832:U:H2'    | 1:1A:3833:C:H6     | 1.81                     | 0.44              |
| 1:1A:4059:C:O2'    | 1:1A:4060:U:H5     | 2.01                     | 0.44              |
| 1:1A:4127:A:C2     | 10:2B:37:LYS:HG2   | 2.53                     | 0.44              |
| 1:1A:4345:C:H2'    | 1:1A:4346:U:C6     | 2.53                     | 0.44              |
| 1:1A:4684:A:C2'    | 1:1A:4685:U:H5'    | 2.48                     | 0.44              |
| 1:1A:4924:C:H2'    | 1:1A:4925:U:C2     | 2.52                     | 0.44              |
| 2:1B:118:C:H2'     | 2:1B:119:U:O4'     | 2.18                     | 0.44              |
| 5:1E:96:PRO:HD3    | 17:2I:156:LEU:HD12 | 1.99                     | 0.44              |
| 8:1H:281:ILE:CG2   | 8:1H:286:LEU:HD21  | 2.48                     | 0.44              |
| 9:2A:47:ARG:O      | 9:2A:50:ILE:HG12   | 2.16                     | 0.44              |
| 12:2D:30:LYS:HE3   | 12:2D:30:LYS:HB3   | 1.76                     | 0.44              |
| 22:2N:102:ARG:HH11 | 22:2N:106:LEU:HD21 | 1.82                     | 0.44              |
| 25:2Q:77:LYS:HE2   | 25:2Q:79:GLN:HB2   | 1.99                     | 0.44              |
| 26:2R:78:LYS:HB2   | 26:2R:99:ILE:O     | 2.18                     | 0.44              |
| 31:2W:18:LEU:O     | 31:2W:22:MET:HG2   | 2.18                     | 0.44              |
| 44:2j:46:LYS:HE3   | 44:2j:46:LYS:HB3   | 1.70                     | 0.44              |
| 47:2m:85:A:H5''    | 76:3N:118:ARG:HE   | 1.82                     | 0.44              |
| 47:2m:398:A:H4'    | 47:2m:399:C:H5''   | 1.97                     | 0.44              |
| 47:2m:793:G:O2'    | 47:2m:794:A:O4'    | 2.34                     | 0.44              |
| 47:2m:976:G:O2'    | 47:2m:977:C:H5'    | 2.18                     | 0.44              |
| 47:2m:1121:G:N3    | 47:2m:1121:G:H2'   | 2.32                     | 0.44              |
| 47:2m:1179:G:N2    | 47:2m:1182:A:OP2   | 2.49                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1452:A:N6    | 47:2m:1473:G:O2'   | 2.51                     | 0.44              |
| 47:2m:1610:G:H2'   | 47:2m:1611:G:C1'   | 2.47                     | 0.44              |
| 47:2m:1693:G:N2    | 47:2m:1834:A:C8    | 2.85                     | 0.44              |
| 47:2m:1780:G:H3'   | 47:2m:1781:A:C8    | 2.53                     | 0.44              |
| 48:2n:65:ILE:HG13  | 48:2n:74:VAL:HG11  | 2.00                     | 0.44              |
| 50:2p:192:TRP:CG   | 50:2p:194:PRO:HD3  | 2.53                     | 0.44              |
| 51:2q:151:ASP:OD1  | 51:2q:152:PRO:HD2  | 2.18                     | 0.44              |
| 51:2q:247:THR:HG23 | 51:2q:250:GLU:OE2  | 2.18                     | 0.44              |
| 54:2t:129:LEU:HB3  | 54:2t:133:GLU:CD   | 2.43                     | 0.44              |
| 54:2t:135:GLU:O    | 54:2t:139:LYS:HG2  | 2.18                     | 0.44              |
| 55:2u:1:MET:HE2    | 55:2u:47:LYS:CB    | 2.48                     | 0.44              |
| 57:2w:17:TYR:CD2   | 57:2w:18:ARG:HG3   | 2.52                     | 0.44              |
| 58:2x:9:SER:HB2    | 58:2x:25:CYS:O     | 2.17                     | 0.44              |
| 59:2y:48:ASN:OD1   | 59:2y:48:ASN:N     | 2.51                     | 0.44              |
| 61:20:107:LEU:CB   | 61:20:113:VAL:HG12 | 2.48                     | 0.44              |
| 62:21:49:LYS:HG2   | 62:21:49:LYS:O     | 2.18                     | 0.44              |
| 69:3G:104:ASP:HA   | 69:3G:129:ALA:O    | 2.18                     | 0.44              |
| 70:3H:7:PHE:CZ     | 70:3H:9:ALA:HB3    | 2.53                     | 0.44              |
| 70:3H:7:PHE:O      | 70:3H:11:GLY:N     | 2.51                     | 0.44              |
| 70:3H:15:LEU:O     | 70:3H:15:LEU:HD13  | 2.18                     | 0.44              |
| 74:3L:60:MET:C     | 74:3L:61:LYS:HD3   | 2.42                     | 0.44              |
| 74:3L:90:ILE:O     | 74:3L:124:MET:HE1  | 2.17                     | 0.44              |
| 75:3M:30:CYS:SG    | 75:3M:61:ILE:HD11  | 2.57                     | 0.44              |
| 76:3N:28:LEU:N     | 76:3N:28:LEU:HD12  | 2.32                     | 0.44              |
| 1:1A:10:A:H2'      | 1:1A:11:G:C8       | 2.53                     | 0.43              |
| 1:1A:39:A:H5''     | 29:2U:35:ALA:HB1   | 2.00                     | 0.43              |
| 1:1A:203:U:O2'     | 1:1A:204:U:H5'     | 2.18                     | 0.43              |
| 1:1A:710:G:H2'     | 1:1A:711:A:H8      | 1.83                     | 0.43              |
| 1:1A:1250:C:O2'    | 1:1A:1251:C:H5'    | 2.18                     | 0.43              |
| 1:1A:1519:C:O2'    | 1:1A:1520:C:H5'    | 2.18                     | 0.43              |
| 1:1A:2320:G:O2'    | 1:1A:2321:G:H5'    | 2.18                     | 0.43              |
| 1:1A:2350:U:OP1    | 1:1A:2351:C:H5''   | 2.17                     | 0.43              |
| 1:1A:2413:U:C2     | 1:1A:2414:G:C8     | 3.06                     | 0.43              |
| 1:1A:3912:U:C2'    | 1:1A:3913:G:H5'    | 2.48                     | 0.43              |
| 1:1A:4143:G:C4     | 1:1A:4145:C:H1'    | 2.52                     | 0.43              |
| 1:1A:4339:A:H2'    | 1:1A:4340:U:H6     | 1.83                     | 0.43              |
| 1:1A:4635:A:H8     | 1:1A:5048:A:H61    | 1.65                     | 0.43              |
| 1:1A:4743:G:H3'    | 1:1A:4744:A:H5''   | 1.99                     | 0.43              |
| 1:1A:4895:C:H4'    | 1:1A:4896:G:O5'    | 2.18                     | 0.43              |
| 1:1A:4927:G:H5''   | 1:1A:4928:C:H5     | 1.82                     | 0.43              |
| 2:1B:61:G:O2'      | 2:1B:62:U:H5'      | 2.17                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:1C:33:G:H4'      | 3:1C:34:U:C5       | 2.53                     | 0.43              |
| 4:1D:65:ASP:OD2    | 4:1D:72:ARG:NE     | 2.43                     | 0.43              |
| 4:1D:96:LEU:HD12   | 4:1D:102:LEU:HD11  | 1.99                     | 0.43              |
| 7:1G:113:PHE:HD2   | 7:1G:115:MET:HE2   | 1.83                     | 0.43              |
| 7:1G:232:THR:HG23  | 7:1G:235:MET:HG3   | 1.99                     | 0.43              |
| 10:2B:39:PHE:CD1   | 10:2B:47:PRO:HD3   | 2.53                     | 0.43              |
| 11:2C:91:LYS:HG3   | 11:2C:183:GLU:HG3  | 2.00                     | 0.43              |
| 12:2D:101:LYS:NZ   | 12:2D:103:LEU:HA   | 2.33                     | 0.43              |
| 12:2D:101:LYS:HD2  | 12:2D:101:LYS:C    | 2.42                     | 0.43              |
| 17:2I:110:PRO:N    | 17:2I:111:PRO:CD   | 2.79                     | 0.43              |
| 20:2L:112:SER:O    | 20:2L:113:LYS:HB2  | 2.18                     | 0.43              |
| 28:2T:18:TYR:HB2   | 28:2T:75:TYR:OH    | 2.18                     | 0.43              |
| 32:2X:42:ALA:HB3   | 32:2X:43:PRO:HD3   | 2.00                     | 0.43              |
| 32:2X:68:LEU:HD13  | 32:2X:108:TYR:HB2  | 2.00                     | 0.43              |
| 46:2L:174:MET:SD   | 46:2L:175:THR:O    | 2.76                     | 0.43              |
| 47:2m:537:C:H3'    | 47:2m:538:U:C5'    | 2.48                     | 0.43              |
| 47:2m:915:G:H21    | 47:2m:915:G:P      | 2.40                     | 0.43              |
| 47:2m:1336:C:H2'   | 47:2m:1337:C:H6    | 1.81                     | 0.43              |
| 47:2m:1533:A:N3    | 47:2m:1533:A:H2'   | 2.32                     | 0.43              |
| 47:2m:1581:C:H3'   | 47:2m:1582:C:C5    | 2.52                     | 0.43              |
| 49:2o:183:GLU:OE2  | 49:2o:187:LYS:HG3  | 2.18                     | 0.43              |
| 49:2o:222:LYS:HA   | 49:2o:222:LYS:HD2  | 1.43                     | 0.43              |
| 52:2r:48:TYR:CE2   | 58:2x:56:LEU:HD13  | 2.53                     | 0.43              |
| 53:2s:129:ILE:HG21 | 53:2s:180:LEU:CD1  | 2.47                     | 0.43              |
| 53:2s:147:LYS:HZ3  | 53:2s:153:LEU:HB2  | 1.83                     | 0.43              |
| 58:2x:17:LYS:HA    | 58:2x:126:ARG:NE   | 2.33                     | 0.43              |
| 58:2x:89:SER:HA    | 58:2x:92:LEU:CD2   | 2.48                     | 0.43              |
| 58:2x:97:GLN:HG2   | 68:3F:60:ARG:CZ    | 2.47                     | 0.43              |
| 58:2x:110:ASP:OD1  | 58:2x:110:ASP:C    | 2.61                     | 0.43              |
| 59:2y:74:GLN:O     | 59:2y:78:ARG:HD3   | 2.18                     | 0.43              |
| 60:2z:121:ARG:HG3  | 60:2z:125:HIS:HD2  | 1.83                     | 0.43              |
| 64:3B:107:ARG:HG2  | 64:3B:112:VAL:HG22 | 1.98                     | 0.43              |
| 65:3C:58:VAL:HG12  | 74:3L:125:LYS:CG   | 2.48                     | 0.43              |
| 68:3F:6:THR:HG23   | 68:3F:313:THR:CG2  | 2.47                     | 0.43              |
| 70:3H:222:GLU:O    | 70:3H:225:GLN:HG2  | 2.18                     | 0.43              |
| 71:3I:32:ILE:HD11  | 71:3I:40:LYS:N     | 2.33                     | 0.43              |
| 71:3I:121:LYS:O    | 71:3I:125:HIS:HB3  | 2.18                     | 0.43              |
| 73:3K:140:LYS:HG3  | 73:3K:141:TYR:N    | 2.33                     | 0.43              |
| 74:3L:42:VAL:O     | 74:3L:42:VAL:HG12  | 2.18                     | 0.43              |
| 77:3O:47:LEU:HG    | 77:3O:47:LEU:O     | 2.18                     | 0.43              |
| 1:1A:203:U:H2'     | 1:1A:204:U:O4'     | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:346:G:OP1    | 27:2S:8:THR:HB     | 2.17                     | 0.43              |
| 1:1A:652:G:C5     | 1:1A:653:U:C5      | 3.06                     | 0.43              |
| 1:1A:1400:G:O2'   | 1:1A:1401:C:H5'    | 2.18                     | 0.43              |
| 1:1A:1463:C:H4'   | 30:2V:29:TYR:O     | 2.18                     | 0.43              |
| 1:1A:1470:G:C2'   | 1:1A:1471:U:H5'    | 2.48                     | 0.43              |
| 1:1A:1537:A:H2'   | 1:1A:1538:U:C6     | 2.53                     | 0.43              |
| 1:1A:1858:A:C2    | 1:1A:1859:C:C5     | 3.06                     | 0.43              |
| 1:1A:1970:A:H5'   | 1:1A:1971:C:H1'    | 2.00                     | 0.43              |
| 1:1A:1999:A:O2'   | 1:1A:2000:G:O4'    | 2.13                     | 0.43              |
| 1:1A:2383:C:N3    | 1:1A:2422:C:H5     | 2.16                     | 0.43              |
| 1:1A:2635:U:H2'   | 1:1A:2636:U:C6     | 2.52                     | 0.43              |
| 1:1A:2787:A:H2    | 1:1A:2801:U:H3     | 1.66                     | 0.43              |
| 1:1A:2888:G:H1'   | 1:1A:3618:C:O2     | 2.19                     | 0.43              |
| 1:1A:3605:C:H2'   | 1:1A:3606:U:O5'    | 2.17                     | 0.43              |
| 1:1A:3973:G:H5''  | 1:1A:4050:A:N6     | 2.33                     | 0.43              |
| 1:1A:4054:C:O2    | 46:2l:207:LYS:HD3  | 2.18                     | 0.43              |
| 1:1A:4399:U:C2'   | 1:1A:4400:G:H5'    | 2.48                     | 0.43              |
| 4:1D:32:VAL:HG12  | 4:1D:163:ARG:CZ    | 2.48                     | 0.43              |
| 5:1E:41:VAL:HA    | 5:1E:186:ASN:O     | 2.18                     | 0.43              |
| 6:1F:261:ASP:O    | 6:1F:265:GLY:N     | 2.48                     | 0.43              |
| 8:1H:165:LEU:HB2  | 8:1H:174:LEU:O     | 2.19                     | 0.43              |
| 8:1H:165:LEU:CD1  | 8:1H:176:THR:HG22  | 2.48                     | 0.43              |
| 8:1H:211:HIS:O    | 8:1H:211:HIS:ND1   | 2.51                     | 0.43              |
| 15:2G:104:MET:SD  | 17:2l:199:HIS:HB3  | 2.57                     | 0.43              |
| 21:2M:98:ARG:HG3  | 21:2M:142:VAL:HG13 | 2.00                     | 0.43              |
| 23:2O:19:LEU:HB2  | 23:2O:73:THR:CG2   | 2.39                     | 0.43              |
| 31:2W:18:LEU:HD23 | 31:2W:18:LEU:HA    | 1.84                     | 0.43              |
| 36:2b:4:ILE:HD11  | 36:2b:56:ARG:HB3   | 2.01                     | 0.43              |
| 36:2b:97:LYS:HD3  | 36:2b:97:LYS:HA    | 1.63                     | 0.43              |
| 36:2b:105:LYS:HE3 | 36:2b:105:LYS:HB3  | 1.89                     | 0.43              |
| 37:2c:33:LEU:HD21 | 37:2c:38:LYS:HG3   | 2.00                     | 0.43              |
| 46:2l:24:LYS:HZ1  | 46:2l:29:LEU:HB2   | 1.83                     | 0.43              |
| 46:2l:73:HIS:HB2  | 46:2l:76:GLU:HB2   | 1.98                     | 0.43              |
| 47:2m:79:A:H2'    | 47:2m:80:G:O5'     | 2.18                     | 0.43              |
| 47:2m:320:G:O6    | 70:3H:186:GLN:NE2  | 2.51                     | 0.43              |
| 47:2m:432:G:O2'   | 47:2m:433:A:H5'    | 2.18                     | 0.43              |
| 47:2m:841:G:N7    | 76:3N:12:PHE:N     | 2.59                     | 0.43              |
| 47:2m:930:C:O2'   | 47:2m:1104:G:OP1   | 2.35                     | 0.43              |
| 47:2m:1110:G:H4'  | 59:2y:124:VAL:CG1  | 2.48                     | 0.43              |
| 47:2m:1304:U:OP1  | 80:3R:95:ARG:HG2   | 2.19                     | 0.43              |
| 47:2m:1510:G:H3'  | 47:2m:1510:G:OP2   | 2.18                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:2m:1592:C:C1'   | 58:2x:44:PRO:HB3  | 2.47                     | 0.43              |
| 48:2n:14:ASP:O     | 48:2n:18:PHE:HD1  | 2.01                     | 0.43              |
| 48:2n:78:SER:HB3   | 48:2n:87:VAL:HG11 | 2.00                     | 0.43              |
| 48:2n:159:ILE:HG22 | 48:2n:159:ILE:O   | 2.18                     | 0.43              |
| 49:2o:139:CYS:HB3  | 49:2o:172:MET:CE  | 2.48                     | 0.43              |
| 51:2q:92:ILE:HG13  | 51:2q:97:GLU:OE1  | 2.18                     | 0.43              |
| 52:2r:56:TYR:HA    | 52:2r:62:ARG:CG   | 2.47                     | 0.43              |
| 52:2r:59:LYS:O     | 52:2r:62:ARG:HB3  | 2.19                     | 0.43              |
| 52:2r:128:ILE:HG12 | 66:3D:23:SER:N    | 2.33                     | 0.43              |
| 52:2r:186:ASN:HA   | 52:2r:191:LYS:CE  | 2.48                     | 0.43              |
| 54:2t:137:LEU:O    | 54:2t:141:ARG:NH1 | 2.50                     | 0.43              |
| 57:2w:20:VAL:HG13  | 57:2w:24:GLN:HB3  | 2.00                     | 0.43              |
| 57:2w:98:ASN:OD1   | 57:2w:100:LYS:HG2 | 2.17                     | 0.43              |
| 65:3C:24:THR:HG23  | 65:3C:72:HIS:O    | 2.17                     | 0.43              |
| 66:3D:43:ILE:HB    | 66:3D:65:ALA:HB1  | 1.99                     | 0.43              |
| 68:3F:37:ASP:C     | 68:3F:38:LYS:HD2  | 2.43                     | 0.43              |
| 70:3H:39:ASP:HB3   | 70:3H:46:LYS:NZ   | 2.33                     | 0.43              |
| 70:3H:44:GLU:HA    | 70:3H:119:LYS:HE3 | 2.00                     | 0.43              |
| 70:3H:118:GLU:OE1  | 70:3H:118:GLU:N   | 2.43                     | 0.43              |
| 73:3K:18:TYR:CD1   | 73:3K:18:TYR:C    | 2.95                     | 0.43              |
| 73:3K:20:ARG:HH21  | 75:3M:56:HIS:CG   | 2.36                     | 0.43              |
| 77:3O:74:SER:HA    | 77:3O:79:ILE:HG22 | 2.00                     | 0.43              |
| 1:1A:425:U:H2'     | 1:1A:426:A:C8     | 2.54                     | 0.43              |
| 1:1A:993:G:O6      | 1:1A:1050:C:H2'   | 2.19                     | 0.43              |
| 1:1A:1241:C:H2'    | 1:1A:1242:G:H1'   | 1.99                     | 0.43              |
| 1:1A:1340:C:H2'    | 1:1A:1341:U:C6    | 2.54                     | 0.43              |
| 1:1A:1871:A:C2'    | 1:1A:1872:G:H5'   | 2.48                     | 0.43              |
| 1:1A:2609:G:H2'    | 1:1A:2610:G:H8    | 1.84                     | 0.43              |
| 1:1A:2634:C:C2     | 1:1A:2635:U:C5    | 3.06                     | 0.43              |
| 1:1A:2706:G:C3'    | 1:1A:2707:U:H5'   | 2.47                     | 0.43              |
| 1:1A:3719:A:C4     | 1:1A:3720:G:C8    | 3.06                     | 0.43              |
| 1:1A:3879:G:O2'    | 1:1A:3881:G:OP2   | 2.27                     | 0.43              |
| 1:1A:3945:A:H2'    | 1:1A:3946:G:C5'   | 2.36                     | 0.43              |
| 1:1A:4555:U:H3'    | 1:1A:4556:U:C5'   | 2.49                     | 0.43              |
| 1:1A:4685:U:H2'    | 1:1A:4686:G:H8    | 1.82                     | 0.43              |
| 1:1A:4734:A:O2'    | 1:1A:4735:G:H5'   | 2.18                     | 0.43              |
| 3:1C:115:G:H2'     | 3:1C:116:C:H6     | 1.83                     | 0.43              |
| 12:2D:47:PRO:HB3   | 12:2D:171:TRP:CZ2 | 2.54                     | 0.43              |
| 13:2E:119:TYR:CE2  | 60:2z:12:ILE:HG23 | 2.53                     | 0.43              |
| 17:2I:179:LYS:HE2  | 17:2I:182:GLU:OE1 | 2.18                     | 0.43              |
| 23:2O:72:VAL:HG21  | 23:2O:83:LEU:HD21 | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:2T:91:LEU:HD12  | 28:2T:113:GLU:OE2  | 2.18                     | 0.43              |
| 29:2U:76:ASP:HB3   | 29:2U:115:GLY:HA3  | 2.00                     | 0.43              |
| 31:2W:11:LEU:C     | 31:2W:14:ILE:HG22  | 2.43                     | 0.43              |
| 43:2i:44:LYS:HE3   | 43:2i:52:THR:HB    | 1.99                     | 0.43              |
| 47:2m:113:G:HO2'   | 47:2m:292:A:H2     | 1.66                     | 0.43              |
| 47:2m:300:U:O2'    | 47:2m:301:A:H5'    | 2.18                     | 0.43              |
| 47:2m:882:U:H4'    | 47:2m:883:U:OP1    | 2.18                     | 0.43              |
| 47:2m:921:G:H3'    | 75:3M:28:ARG:NH1   | 2.32                     | 0.43              |
| 47:2m:1097:G:H4'   | 48:2n:32:PHE:CD1   | 2.53                     | 0.43              |
| 47:2m:1129:G:H2'   | 47:2m:1130:G:C1'   | 2.48                     | 0.43              |
| 47:2m:1174:U:H2'   | 47:2m:1175:G:C8    | 2.53                     | 0.43              |
| 47:2m:1220:A:H2'   | 47:2m:1221:G:O4'   | 2.17                     | 0.43              |
| 47:2m:1304:U:OP2   | 80:3R:95:ARG:HD3   | 2.19                     | 0.43              |
| 47:2m:1478:U:H2'   | 47:2m:1479:G:C8    | 2.53                     | 0.43              |
| 47:2m:1605:G:H2'   | 47:2m:1606:G:C1'   | 2.49                     | 0.43              |
| 48:2n:53:ARG:HB3   | 63:3A:83:PHE:HE2   | 1.83                     | 0.43              |
| 48:2n:148:CYS:SG   | 48:2n:160:ALA:HB1  | 2.57                     | 0.43              |
| 50:2p:65:ARG:HA    | 50:2p:68:GLU:CD    | 2.43                     | 0.43              |
| 50:2p:158:ILE:HG13 | 50:2p:164:VAL:CG1  | 2.48                     | 0.43              |
| 51:2q:94:LYS:HG2   | 76:3N:16:ARG:HG3   | 2.00                     | 0.43              |
| 51:2q:246:LEU:HA   | 51:2q:250:GLU:OE2  | 2.19                     | 0.43              |
| 52:2r:19:LEU:CD2   | 52:2r:23:TRP:HB2   | 2.47                     | 0.43              |
| 52:2r:186:ASN:HA   | 52:2r:191:LYS:HE2  | 1.99                     | 0.43              |
| 57:2w:18:ARG:HD3   | 60:2z:88:LYS:HG2   | 2.00                     | 0.43              |
| 58:2x:111:ILE:HA   | 58:2x:114:GLN:CG   | 2.47                     | 0.43              |
| 59:2y:36:GLU:C     | 59:2y:36:GLU:OE1   | 2.62                     | 0.43              |
| 59:2y:97:GLU:OE1   | 59:2y:120:THR:HG23 | 2.17                     | 0.43              |
| 60:2z:10:GLN:NE2   | 60:2z:57:GLY:HA2   | 2.27                     | 0.43              |
| 68:3F:121:VAL:HG21 | 68:3F:165:ILE:HG21 | 1.99                     | 0.43              |
| 68:3F:247:TRP:CD1  | 68:3F:247:TRP:N    | 2.86                     | 0.43              |
| 69:3G:103:LYS:O    | 69:3G:130:ILE:HD12 | 2.19                     | 0.43              |
| 76:3N:23:MET:SD    | 76:3N:25:ILE:CG1   | 3.07                     | 0.43              |
| 1:1A:710:G:O2'     | 1:1A:711:A:H5'     | 2.18                     | 0.43              |
| 1:1A:1281:G:N1     | 8:1H:128:HIS:HB2   | 2.32                     | 0.43              |
| 1:1A:2418:A:C5     | 1:1A:2419:C:C5     | 3.06                     | 0.43              |
| 1:1A:2781:G:HO2'   | 1:1A:2782:U:H5'    | 1.80                     | 0.43              |
| 1:1A:3712:A:H3'    | 1:1A:3712:A:N3     | 2.34                     | 0.43              |
| 1:1A:3870:C:H5'    | 5:1E:261:ARG:NH1   | 2.34                     | 0.43              |
| 1:1A:4251:A:H2'    | 1:1A:4252:C:C6     | 2.53                     | 0.43              |
| 1:1A:4356:G:C2     | 1:1A:4357:G:C8     | 3.07                     | 0.43              |
| 1:1A:4440:G:C4     | 1:1A:4441:A:C8     | 3.06                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:4869:U:C2'    | 1:1A:4870:G:C5'    | 2.95                     | 0.43              |
| 1:1A:4928:C:O2'    | 15:2G:118:MET:HE2  | 2.18                     | 0.43              |
| 3:1C:68:G:OP2      | 38:2d:87:LYS:HD3   | 2.19                     | 0.43              |
| 6:1F:149:GLU:O     | 6:1F:150:LEU:C     | 2.62                     | 0.43              |
| 10:2B:138:ALA:HB2  | 10:2B:194:VAL:HG11 | 1.99                     | 0.43              |
| 11:2C:16:VAL:HG11  | 11:2C:85:THR:CG2   | 2.49                     | 0.43              |
| 12:2D:190:LEU:HB3  | 12:2D:197:VAL:HG21 | 2.01                     | 0.43              |
| 13:2E:56:THR:CB    | 13:2E:63:ARG:HA    | 2.35                     | 0.43              |
| 23:2O:91:LEU:HD13  | 23:2O:96:LEU:HB2   | 1.99                     | 0.43              |
| 23:2O:103:VAL:HG21 | 23:2O:113:ARG:CZ   | 2.48                     | 0.43              |
| 28:2T:22:LYS:HE3   | 28:2T:129:TRP:O    | 2.18                     | 0.43              |
| 32:2X:33:ILE:HD13  | 32:2X:33:ILE:HA    | 1.76                     | 0.43              |
| 34:2Z:105:LEU:HG   | 34:2Z:105:LEU:O    | 2.18                     | 0.43              |
| 46:2l:160:LYS:HG3  | 46:2l:161:LYS:N    | 2.27                     | 0.43              |
| 47:2m:330:G:H5'    | 47:2m:331:C:OP2    | 2.19                     | 0.43              |
| 47:2m:678:U:H2'    | 47:2m:679:A:H8     | 1.82                     | 0.43              |
| 47:2m:1299:A:N7    | 47:2m:1301:A:H5''  | 2.34                     | 0.43              |
| 47:2m:1330:G:N7    | 47:2m:1492:U:H3'   | 2.34                     | 0.43              |
| 47:2m:1649:U:C5'   | 58:2x:128:GLU:HB2  | 2.49                     | 0.43              |
| 48:2n:146:ALA:HB3  | 48:2n:157:VAL:HG11 | 2.00                     | 0.43              |
| 49:2o:25:PHE:CE1   | 74:3L:88:LEU:HD21  | 2.54                     | 0.43              |
| 49:2o:34:LYS:HZ2   | 49:2o:43:ASN:HB2   | 1.82                     | 0.43              |
| 49:2o:131:ASP:O    | 49:2o:221:PRO:HB3  | 2.18                     | 0.43              |
| 49:2o:150:ILE:HD13 | 59:2y:132:ARG:NH1  | 2.33                     | 0.43              |
| 49:2o:208:HIS:ND1  | 49:2o:208:HIS:N    | 2.65                     | 0.43              |
| 50:2p:14:ASP:O     | 50:2p:18:LYS:HG3   | 2.18                     | 0.43              |
| 50:2p:54:ARG:CD    | 50:2p:57:ASN:HB2   | 2.49                     | 0.43              |
| 52:2r:167:LYS:O    | 52:2r:167:LYS:HG2  | 2.17                     | 0.43              |
| 52:2r:182:LYS:HE2  | 52:2r:184:SER:HB3  | 2.01                     | 0.43              |
| 53:2s:20:GLU:CD    | 53:2s:23:ILE:HD12  | 2.42                     | 0.43              |
| 53:2s:187:PHE:O    | 53:2s:188:GLU:HG3  | 2.18                     | 0.43              |
| 55:2u:21:MET:SD    | 55:2u:69:TRP:HE3   | 2.40                     | 0.43              |
| 57:2w:15:PHE:CE2   | 57:2w:109:PRO:HB2  | 2.53                     | 0.43              |
| 57:2w:56:LEU:CD1   | 57:2w:60:LEU:HD21  | 2.48                     | 0.43              |
| 59:2y:45:LYS:HE3   | 59:2y:49:LYS:NZ    | 2.33                     | 0.43              |
| 60:2z:118:ARG:CZ   | 60:2z:118:ARG:HB2  | 2.48                     | 0.43              |
| 61:20:22:LEU:HB3   | 61:20:28:LEU:HD23  | 1.99                     | 0.43              |
| 62:21:29:VAL:HA    | 62:21:32:LEU:HB3   | 2.01                     | 0.43              |
| 64:3B:81:ILE:HD11  | 64:3B:102:VAL:HG11 | 2.00                     | 0.43              |
| 65:3C:45:VAL:HB    | 65:3C:50:VAL:HG22  | 2.00                     | 0.43              |
| 69:3G:92:GLU:OE1   | 69:3G:92:GLU:N     | 2.31                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 70:3H:147:LEU:HB3 | 70:3H:151:ASP:HB2  | 2.00                     | 0.43              |
| 71:3I:29:LEU:HD12 | 71:3I:29:LEU:O     | 2.18                     | 0.43              |
| 76:3N:41:ARG:HB2  | 76:3N:55:ILE:HG21  | 2.00                     | 0.43              |
| 77:3O:97:ILE:HD12 | 77:3O:111:ARG:HA   | 2.01                     | 0.43              |
| 1:1A:67:C:H41     | 1:1A:326:C:H5'     | 1.84                     | 0.43              |
| 1:1A:216:C:H5'    | 1:1A:219:G:C2      | 2.54                     | 0.43              |
| 1:1A:1179:U:C4'   | 1:1A:1180:C:H5''   | 2.48                     | 0.43              |
| 1:1A:1187:G:H2'   | 1:1A:1188:C:C6     | 2.54                     | 0.43              |
| 1:1A:1270:A:H5'   | 1:1A:1271:G:OP1    | 2.19                     | 0.43              |
| 1:1A:1804:A:O4'   | 1:1A:1806:G:C8     | 2.72                     | 0.43              |
| 1:1A:2789:A:HO2'  | 40:2f:45:ARG:NH2   | 1.97                     | 0.43              |
| 1:1A:2846:G:O2'   | 1:1A:2847:G:H5'    | 2.18                     | 0.43              |
| 1:1A:3662:A:H5'   | 1:1A:3664:G:O4'    | 2.17                     | 0.43              |
| 1:1A:3923:A:H2'   | 1:1A:3924:C:C6     | 2.53                     | 0.43              |
| 1:1A:4063:U:H3'   | 1:1A:4064:C:C5     | 2.54                     | 0.43              |
| 1:1A:4383:U:H2'   | 1:1A:4384:U:C6     | 2.53                     | 0.43              |
| 1:1A:4464:A:H4'   | 1:1A:4465:U:OP1    | 2.18                     | 0.43              |
| 2:1B:60:G:C2      | 2:1B:61:G:C8       | 3.07                     | 0.43              |
| 3:1C:92:U:H2'     | 3:1C:93:C:O4'      | 2.17                     | 0.43              |
| 7:1G:86:TYR:CD1   | 7:1G:86:TYR:O      | 2.71                     | 0.43              |
| 17:2I:72:HIS:O    | 17:2I:74:ARG:NH1   | 2.51                     | 0.43              |
| 27:2S:47:MET:HE3  | 27:2S:122:LYS:HD2  | 2.00                     | 0.43              |
| 28:2T:29:ILE:CG2  | 28:2T:32:GLY:H     | 2.30                     | 0.43              |
| 32:2X:23:ARG:HG2  | 32:2X:121:ASN:OD1  | 2.18                     | 0.43              |
| 47:2m:123:G:H5'   | 47:2m:124:U:OP2    | 2.17                     | 0.43              |
| 47:2m:912:C:O2'   | 47:2m:913:A:O5'    | 2.34                     | 0.43              |
| 47:2m:1079:C:O2'  | 47:2m:1182:A:N1    | 2.46                     | 0.43              |
| 47:2m:1119:A:H5'  | 78:3P:72:ARG:HH12  | 1.83                     | 0.43              |
| 47:2m:1616:U:O2'  | 47:2m:1617:G:H5'   | 2.19                     | 0.43              |
| 47:2m:1648:G:H22  | 47:2m:1674:G:H3'   | 1.83                     | 0.43              |
| 47:2m:1696:C:O2'  | 47:2m:1699:A:O2'   | 2.36                     | 0.43              |
| 47:2m:1713:C:H2'  | 47:2m:1714:U:C6    | 2.53                     | 0.43              |
| 47:2m:1868:U:C2   | 65:3C:100:ARG:HD3  | 2.54                     | 0.43              |
| 48:2n:40:LYS:NZ   | 59:2y:101:ASP:HB3  | 2.34                     | 0.43              |
| 50:2p:11:PHE:HE2  | 62:21:84:ILE:HG23  | 1.84                     | 0.43              |
| 50:2p:205:PRO:HA  | 59:2y:42:PRO:HG2   | 2.00                     | 0.43              |
| 51:2q:49:ARG:HG3  | 51:2q:55:ALA:O     | 2.19                     | 0.43              |
| 51:2q:103:TYR:CG  | 51:2q:189:LEU:HD11 | 2.54                     | 0.43              |
| 51:2q:121:TYR:HD2 | 51:2q:161:GLN:HG2  | 1.82                     | 0.43              |
| 53:2s:9:VAL:O     | 53:2s:9:VAL:HG23   | 2.18                     | 0.43              |
| 54:2t:165:GLN:NE2 | 54:2t:195:LEU:HD21 | 2.32                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:2u:27:VAL:HG12  | 55:2u:43:LEU:HD12  | 2.01                     | 0.43              |
| 55:2u:35:LEU:HD21  | 55:2u:38:LYS:N     | 2.31                     | 0.43              |
| 58:2x:21:ALA:CB    | 58:2x:72:VAL:HG13  | 2.38                     | 0.43              |
| 59:2y:44:LYS:O     | 59:2y:48:ASN:OD1   | 2.36                     | 0.43              |
| 62:21:29:VAL:HG23  | 62:21:85:HIS:CG    | 2.53                     | 0.43              |
| 68:3F:18:VAL:HG21  | 68:3F:307:VAL:CG2  | 2.49                     | 0.43              |
| 68:3F:172:LYS:HG2  | 68:3F:194:TYR:HA   | 2.01                     | 0.43              |
| 68:3F:173:LEU:HD23 | 68:3F:187:ASN:HD21 | 1.83                     | 0.43              |
| 69:3G:130:ILE:HG13 | 69:3G:131:GLY:N    | 2.33                     | 0.43              |
| 69:3G:178:HIS:HB2  | 69:3G:220:ASP:OD1  | 2.19                     | 0.43              |
| 71:3I:12:THR:O     | 71:3I:45:ARG:HA    | 2.18                     | 0.43              |
| 71:3I:124:HIS:CD2  | 79:3Q:31:ARG:HE    | 2.36                     | 0.43              |
| 74:3L:131:ASP:OD1  | 74:3L:133:THR:OG1  | 2.33                     | 0.43              |
| 75:3M:44:HIS:NE2   | 75:3M:112:ASP:OD2  | 2.51                     | 0.43              |
| 1:1A:352:G:O2'     | 3:1C:22:U:O4       | 2.32                     | 0.43              |
| 1:1A:759:G:C2'     | 1:1A:760:G:H5'     | 2.39                     | 0.43              |
| 1:1A:1218:G:C3'    | 1:1A:1219:G:H5''   | 2.40                     | 0.43              |
| 1:1A:1239:C:OP1    | 30:2V:92:LYS:NZ    | 2.52                     | 0.43              |
| 1:1A:1577:G:H3'    | 1:1A:1577:G:N3     | 2.34                     | 0.43              |
| 1:1A:1580:C:C2'    | 1:1A:1581:G:H5'    | 2.48                     | 0.43              |
| 1:1A:1806:G:O2'    | 1:1A:1807:C:H5'    | 2.18                     | 0.43              |
| 1:1A:1929:A:H2'    | 1:1A:1929:A:N3     | 2.33                     | 0.43              |
| 1:1A:2389:A:O2'    | 1:1A:2390:G:O5'    | 2.36                     | 0.43              |
| 1:1A:3677:U:OP2    | 1:1A:3678:G:O2'    | 2.31                     | 0.43              |
| 1:1A:4873:G:N7     | 17:2I:203:VAL:HG23 | 2.34                     | 0.43              |
| 1:1A:4990:C:H3'    | 1:1A:4991:U:H5''   | 1.99                     | 0.43              |
| 4:1D:39:GLY:HA2    | 4:1D:93:LYS:CG     | 2.49                     | 0.43              |
| 7:1G:119:TYR:OH    | 7:1G:139:PRO:O     | 2.33                     | 0.43              |
| 7:1G:178:LYS:HE2   | 7:1G:179:ARG:NH1   | 2.34                     | 0.43              |
| 11:2C:88:PHE:CE2   | 11:2C:151:ILE:HB   | 2.54                     | 0.43              |
| 13:2E:83:LEU:HD12  | 13:2E:170:TYR:CZ   | 2.53                     | 0.43              |
| 17:2I:165:LYS:HB2  | 17:2I:165:LYS:HE3  | 1.77                     | 0.43              |
| 20:2L:169:ALA:HA   | 20:2L:172:ARG:NH2  | 2.33                     | 0.43              |
| 23:2O:91:LEU:HB3   | 23:2O:97:ARG:HG3   | 2.00                     | 0.43              |
| 24:2P:87:SER:CA    | 24:2P:97:TYR:HB3   | 2.48                     | 0.43              |
| 30:2V:95:ARG:O     | 30:2V:99:ILE:HG13  | 2.19                     | 0.43              |
| 42:2h:11:ARG:NH2   | 47:2m:1184:G:OP1   | 2.52                     | 0.43              |
| 46:2l:143:ASN:H    | 46:2l:148:VAL:CG1  | 2.30                     | 0.43              |
| 47:2m:113:G:C2     | 47:2m:292:A:H1'    | 2.54                     | 0.43              |
| 47:2m:872:A:O2'    | 47:2m:873:G:O5'    | 2.36                     | 0.43              |
| 47:2m:877:C:C5     | 47:2m:879:C:H5''   | 2.54                     | 0.43              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 47:2m:899:U:H3'    | 47:2m:900:C:C5'      | 2.48                     | 0.43              |
| 47:2m:1138:C:C2    | 63:3A:61:ARG:HD2     | 2.53                     | 0.43              |
| 47:2m:1344:A:H4'   | 47:2m:1345:G:OP1     | 2.18                     | 0.43              |
| 47:2m:1544:C:H4'   | 58:2x:80:GLN:HE22    | 1.82                     | 0.43              |
| 47:2m:1865:C:C5    | 65:3C:92:ARG:HB3     | 2.54                     | 0.43              |
| 48:2n:34:MET:HE2   | 48:2n:149:ASN:C      | 2.44                     | 0.43              |
| 48:2n:42:LYS:HD2   | 48:2n:48:ILE:HD11    | 2.00                     | 0.43              |
| 49:2o:183:GLU:OE2  | 49:2o:187:LYS:HD2    | 2.19                     | 0.43              |
| 49:2o:185:VAL:HA   | 49:2o:188:LEU:CD2    | 2.49                     | 0.43              |
| 50:2p:72:VAL:HG13  | 55:2u:20:VAL:CG2     | 2.49                     | 0.43              |
| 51:2q:179:ASN:O    | 51:2q:194:VAL:HA     | 2.17                     | 0.43              |
| 52:2r:200:ALA:HA   | 52:2r:203:ASN:ND2    | 2.34                     | 0.43              |
| 53:2s:69:LEU:HD13  | 53:2s:96:ALA:HB2     | 2.00                     | 0.43              |
| 53:2s:130:LEU:HD13 | 53:2s:177:TYR:CZ     | 2.53                     | 0.43              |
| 53:2s:152:ARG:NH2  | 75:3M:35:VAL:HG11    | 2.34                     | 0.43              |
| 55:2u:37:ASP:HB2   | 55:2u:38:LYS:HZ3     | 1.83                     | 0.43              |
| 56:2v:59:LYS:HA    | 56:2v:66:VAL:CG1     | 2.48                     | 0.43              |
| 60:2z:10:GLN:NE2   | 60:2z:22:GLY:HA3     | 2.33                     | 0.43              |
| 64:3B:115:ILE:CG2  | 64:3B:118:VAL:HB     | 2.49                     | 0.43              |
| 66:3D:24:GLN:N     | 66:3D:24:GLN:CD      | 2.76                     | 0.43              |
| 76:3N:10:ARG:HH11  | 76:3N:26:ASP:CG      | 2.25                     | 0.43              |
| 76:3N:58:PHE:CD1   | 76:3N:58:PHE:N       | 2.86                     | 0.43              |
| 76:3N:110:ARG:HG2  | 76:3N:113[B]:ARG:NH2 | 2.33                     | 0.43              |
| 1:1A:26:C:H42      | 1:1A:56:A:N6         | 2.17                     | 0.43              |
| 1:1A:164:G:H2'     | 1:1A:165:A:H8        | 1.84                     | 0.43              |
| 1:1A:305:A:P       | 16:2H:15:GLN:HE22    | 2.40                     | 0.43              |
| 1:1A:457:G:OP1     | 8:1H:115:TYR:CD2     | 2.72                     | 0.43              |
| 1:1A:653:U:H2'     | 1:1A:654:C:C6        | 2.54                     | 0.43              |
| 1:1A:956:A:O2'     | 1:1A:2077:C:OP1      | 2.33                     | 0.43              |
| 1:1A:959:G:C8      | 8:1H:123:ARG:HG2     | 2.53                     | 0.43              |
| 1:1A:1315:C:H2'    | 1:1A:1316:G:C8       | 2.53                     | 0.43              |
| 1:1A:1751:A:H2'    | 1:1A:1752:G:H8       | 1.83                     | 0.43              |
| 1:1A:2299:G:HO2'   | 1:1A:2300:A:P        | 2.29                     | 0.43              |
| 1:1A:2436:U:H4'    | 1:1A:2437:C:OP2      | 2.18                     | 0.43              |
| 1:1A:3823:G:HO2'   | 1:1A:3824:A:H8       | 1.62                     | 0.43              |
| 1:1A:3911:C:C2     | 1:1A:3912:U:C5       | 3.07                     | 0.43              |
| 1:1A:4323:A:N6     | 7:1G:153:THR:HG21    | 2.33                     | 0.43              |
| 1:1A:4331:G:O2'    | 1:1A:4332:C:OP1      | 2.36                     | 0.43              |
| 1:1A:4453:C:C2'    | 1:1A:4454:G:H5'      | 2.49                     | 0.43              |
| 1:1A:4901:G:H3'    | 1:1A:4901:G:P        | 2.58                     | 0.43              |
| 3:1C:140:C:H2'     | 3:1C:141:C:C6        | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:146:GLU:HB2   | 6:1F:175:LYS:HB3   | 2.00                     | 0.43              |
| 6:1F:205:ARG:HA    | 6:1F:205:ARG:HD3   | 1.78                     | 0.43              |
| 15:2G:33:GLN:CB    | 21:2M:145:PHE:HZ   | 2.32                     | 0.43              |
| 19:2K:64:SER:OG    | 19:2K:89:ASP:OD2   | 2.34                     | 0.43              |
| 19:2K:69:LYS:HA    | 19:2K:69:LYS:HD3   | 1.82                     | 0.43              |
| 21:2M:96:GLU:HG3   | 21:2M:139:ARG:CG   | 2.41                     | 0.43              |
| 23:2O:100:LEU:HD23 | 23:2O:112:LEU:HD23 | 1.99                     | 0.43              |
| 24:2P:92:ASP:OD1   | 24:2P:92:ASP:N     | 2.52                     | 0.43              |
| 25:2Q:91:MET:HA    | 25:2Q:91:MET:CE    | 2.42                     | 0.43              |
| 25:2Q:106:GLU:OE1  | 25:2Q:109:ILE:HG21 | 2.18                     | 0.43              |
| 26:2R:39:LYS:H     | 26:2R:39:LYS:HG2   | 1.65                     | 0.43              |
| 39:2e:9:LYS:HG3    | 39:2e:10:ASP:H     | 1.82                     | 0.43              |
| 45:2k:35:ARG:O     | 45:2k:35:ARG:HG3   | 2.18                     | 0.43              |
| 47:2m:11:A:N1      | 47:2m:1200:A:H2    | 2.16                     | 0.43              |
| 47:2m:434:G:P      | 54:2t:25:ARG:HH22  | 2.41                     | 0.43              |
| 47:2m:1043:G:N2    | 47:2m:1074:C:N3    | 2.67                     | 0.43              |
| 47:2m:1102:G:C6    | 47:2m:1131:G:C6    | 3.06                     | 0.43              |
| 47:2m:1581:C:H3'   | 47:2m:1582:C:H5    | 1.84                     | 0.43              |
| 47:2m:1744:G:H8    | 47:2m:1744:G:OP2   | 2.01                     | 0.43              |
| 48:2n:53:ARG:HG2   | 48:2n:53:ARG:H     | 1.70                     | 0.43              |
| 50:2p:226:GLN:NE2  | 68:3F:186:THR:HG23 | 2.33                     | 0.43              |
| 51:2q:180:LEU:CD2  | 51:2q:228:ILE:HG13 | 2.49                     | 0.43              |
| 52:2r:175:ASP:HA   | 52:2r:178:ILE:CG1  | 2.48                     | 0.43              |
| 53:2s:7:LYS:HZ1    | 53:2s:24:SER:H     | 1.65                     | 0.43              |
| 53:2s:31:GLU:C     | 53:2s:32:MET:HE2   | 2.43                     | 0.43              |
| 53:2s:65:PRO:HB2   | 53:2s:68:GLN:HG3   | 1.99                     | 0.43              |
| 53:2s:148:LEU:HA   | 75:3M:42:MET:SD    | 2.58                     | 0.43              |
| 54:2t:205:ARG:HG3  | 54:2t:205:ARG:HH11 | 1.84                     | 0.43              |
| 55:2u:85:LEU:HG    | 55:2u:86:PRO:HD2   | 2.00                     | 0.43              |
| 57:2w:38:SER:OG    | 57:2w:39:ALA:N     | 2.51                     | 0.43              |
| 57:2w:101:THR:OG1  | 57:2w:102:PHE:N    | 2.48                     | 0.43              |
| 60:2z:138:THR:O    | 60:2z:139:THR:HG23 | 2.19                     | 0.43              |
| 64:3B:9:THR:O      | 64:3B:13:LEU:HG    | 2.19                     | 0.43              |
| 68:3F:242:SER:HB3  | 68:3F:245:ARG:C    | 2.43                     | 0.43              |
| 69:3G:135:GLY:O    | 69:3G:164:PRO:HA   | 2.19                     | 0.43              |
| 70:3H:139:SER:HA   | 70:3H:142:ARG:CD   | 2.48                     | 0.43              |
| 71:3I:127:ARG:NH2  | 71:3I:145:PRO:HG2  | 2.33                     | 0.43              |
| 1:1A:11:G:H2'      | 1:1A:12:A:C8       | 2.54                     | 0.43              |
| 1:1A:48:G:HO2'     | 1:1A:49:U:P        | 2.41                     | 0.43              |
| 1:1A:66:A:H5''     | 1:1A:328:A:H5'     | 2.01                     | 0.43              |
| 1:1A:143:C:H5''    | 1:1A:144:G:OP1     | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:150:U:H4'     | 1:1A:151:G:OP2     | 2.18                     | 0.43              |
| 1:1A:306:A:O2'     | 1:1A:307:A:H5'     | 2.18                     | 0.43              |
| 1:1A:481:G:C6      | 1:1A:674:G:C6      | 3.07                     | 0.43              |
| 1:1A:1380:G:H4'    | 1:1A:1381:U:H6     | 1.83                     | 0.43              |
| 1:1A:1693:U:P      | 19:2K:143:ARG:HH22 | 2.42                     | 0.43              |
| 1:1A:2459:G:H2'    | 1:1A:2461:G:OP2    | 2.18                     | 0.43              |
| 1:1A:2487:G:OP2    | 1:1A:2487:G:H2'    | 2.19                     | 0.43              |
| 1:1A:2559:G:H2'    | 1:1A:2560:C:H6     | 1.79                     | 0.43              |
| 1:1A:2621:A:H2'    | 1:1A:2622:G:H8     | 1.83                     | 0.43              |
| 1:1A:3654:G:H22    | 1:1A:3817:A:H2     | 1.67                     | 0.43              |
| 1:1A:3924:C:O2'    | 1:1A:3925:U:H5'    | 2.19                     | 0.43              |
| 1:1A:4324:A:O2'    | 1:1A:4325:A:H5'    | 2.18                     | 0.43              |
| 1:1A:4941:G:OP1    | 8:1H:219:LYS:HE3   | 2.19                     | 0.43              |
| 2:1B:33:U:C2'      | 2:1B:34:C:O5'      | 2.67                     | 0.43              |
| 3:1C:155:C:H2'     | 3:1C:156:U:O4'     | 2.19                     | 0.43              |
| 5:1E:14:LEU:HD22   | 5:1E:17:LEU:HD13   | 2.01                     | 0.43              |
| 7:1G:164:LYS:CA    | 7:1G:167:VAL:HG22  | 2.48                     | 0.43              |
| 10:2B:120:LYS:HA   | 10:2B:123:ALA:HB3  | 2.01                     | 0.43              |
| 10:2B:136:LEU:HD13 | 10:2B:193:LEU:HD13 | 2.00                     | 0.43              |
| 12:2D:42:LYS:HB2   | 12:2D:45:GLU:HG3   | 2.01                     | 0.43              |
| 15:2G:37:LEU:HD12  | 15:2G:48:GLN:O     | 2.19                     | 0.43              |
| 21:2M:84:TYR:HE1   | 21:2M:93:MET:HE3   | 1.83                     | 0.43              |
| 24:2P:48:ARG:HG2   | 24:2P:49:LEU:H     | 1.84                     | 0.43              |
| 33:2Y:35:TRP:CE2   | 33:2Y:56:PRO:HD2   | 2.54                     | 0.43              |
| 38:2d:67:LEU:HD23  | 38:2d:67:LEU:HA    | 1.85                     | 0.43              |
| 46:2l:12:GLU:O     | 46:2l:217:TYR:HB3  | 2.19                     | 0.43              |
| 47:2m:53:C:O2      | 47:2m:53:C:H2'     | 2.17                     | 0.43              |
| 47:2m:118:C:H2'    | 47:2m:119:U:H5'    | 2.01                     | 0.43              |
| 47:2m:309:G:H2'    | 47:2m:310:C:H1'    | 1.99                     | 0.43              |
| 47:2m:562:U:H2'    | 47:2m:563:G:H8     | 1.80                     | 0.43              |
| 47:2m:569:A:C2     | 47:2m:570:C:C6     | 3.07                     | 0.43              |
| 47:2m:888:U:HO2'   | 47:2m:889:U:H3'    | 1.84                     | 0.43              |
| 47:2m:1110:G:H4'   | 59:2y:124:VAL:HG11 | 2.01                     | 0.43              |
| 47:2m:1654:G:N2    | 47:2m:1671:G:N2    | 2.66                     | 0.43              |
| 47:2m:1677:U:C4    | 47:2m:1678:A:H2    | 2.36                     | 0.43              |
| 47:2m:1866:A:H5'   | 65:3C:95:ARG:HG2   | 2.01                     | 0.43              |
| 48:2n:29:ASN:OD1   | 48:2n:151:ASP:HB3  | 2.18                     | 0.43              |
| 48:2n:104:THR:HG23 | 48:2n:107:THR:OG1  | 2.19                     | 0.43              |
| 50:2p:217:ILE:CG2  | 50:2p:218:LEU:HD23 | 2.44                     | 0.43              |
| 51:2q:149:TYR:N    | 51:2q:150:PRO:HD3  | 2.34                     | 0.43              |
| 53:2s:147:LYS:HE2  | 53:2s:151:SER:OG   | 2.18                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 57:2w:85:ILE:CD1   | 57:2w:116:LEU:HA  | 2.48                     | 0.43              |
| 59:2y:47:ARG:HE    | 59:2y:47:ARG:HB3  | 1.68                     | 0.43              |
| 59:2y:116:ASN:OD1  | 59:2y:117:LEU:N   | 2.50                     | 0.43              |
| 65:3C:25:ASN:HD21  | 65:3C:77:CYS:CB   | 2.29                     | 0.43              |
| 68:3F:42:MET:HE2   | 68:3F:57:ARG:HB3  | 2.00                     | 0.43              |
| 69:3G:77:SER:HB2   | 69:3G:79:GLU:OE1  | 2.18                     | 0.43              |
| 69:3G:204:ILE:HD11 | 69:3G:219:ILE:O   | 2.19                     | 0.43              |
| 70:3H:49:VAL:HG22  | 70:3H:115:LYS:HB3 | 2.01                     | 0.43              |
| 70:3H:166:GLY:C    | 70:3H:167:LYS:HD2 | 2.43                     | 0.43              |
| 75:3M:69:LEU:HD21  | 75:3M:72:CYS:SG   | 2.58                     | 0.43              |
| 76:3N:127:ALA:O    | 76:3N:131:PRO:HD2 | 2.17                     | 0.43              |
| 77:3O:63:PRO:HB3   | 77:3O:97:ILE:HG12 | 1.99                     | 0.43              |
| 78:3P:30:SER:HB2   | 78:3P:47:PHE:CE1  | 2.54                     | 0.43              |
| 1:1A:121:A:N3      | 1:1A:121:A:C2'    | 2.82                     | 0.43              |
| 1:1A:302:C:H2'     | 1:1A:303:C:H6     | 1.83                     | 0.43              |
| 1:1A:677:G:H2'     | 1:1A:678:C:H6     | 1.82                     | 0.43              |
| 1:1A:1426:G:N1     | 1:1A:1458:C:OP2   | 2.37                     | 0.43              |
| 1:1A:1855:G:C6     | 1:1A:1880:G:N2    | 2.86                     | 0.43              |
| 1:1A:1883:G:O6     | 1:1A:1896:A:H2    | 2.01                     | 0.43              |
| 1:1A:2055:G:H3'    | 1:1A:2056:G:C5'   | 2.49                     | 0.43              |
| 1:1A:2721:G:H2'    | 1:1A:2722:G:H5'   | 2.01                     | 0.43              |
| 1:1A:3747:A:N7     | 4:1D:245:ARG:HD3  | 2.34                     | 0.43              |
| 1:1A:3900:G:OP1    | 1:1A:3901:A:H4'   | 2.18                     | 0.43              |
| 1:1A:3914:U:H5'    | 1:1A:3915:U:OP1   | 2.19                     | 0.43              |
| 1:1A:3974:G:N2     | 1:1A:4051:C:OP1   | 2.52                     | 0.43              |
| 1:1A:4165:C:O2'    | 1:1A:4166:G:H5'   | 2.18                     | 0.43              |
| 1:1A:4194:U:H5'    | 30:2V:3:LYS:CD    | 2.49                     | 0.43              |
| 1:1A:4480:A:O2'    | 1:1A:4481:U:H5'   | 2.18                     | 0.43              |
| 1:1A:4510:A:O2'    | 1:1A:4511:A:H5'   | 2.19                     | 0.43              |
| 1:1A:4521:U:H1'    | 5:1E:253:CYS:SG   | 2.59                     | 0.43              |
| 1:1A:4589:A:N1     | 1:1A:4621:C:O2'   | 2.46                     | 0.43              |
| 1:1A:4860:G:O2'    | 1:1A:4861:G:OP1   | 2.29                     | 0.43              |
| 4:1D:46:LYS:HG3    | 4:1D:62:VAL:CG2   | 2.49                     | 0.43              |
| 8:1H:138:ARG:HD2   | 8:1H:170:SER:C    | 2.43                     | 0.43              |
| 9:2A:182:TYR:CZ    | 9:2A:203:GLU:HG2  | 2.54                     | 0.43              |
| 11:2C:91:LYS:HG3   | 11:2C:183:GLU:CG  | 2.48                     | 0.43              |
| 12:2D:34:PHE:HA    | 12:2D:89:VAL:CG2  | 2.49                     | 0.43              |
| 13:2E:88:LYS:HG3   | 13:2E:89:VAL:N    | 2.34                     | 0.43              |
| 16:2H:96:ARG:NH1   | 16:2H:100:SER:OG  | 2.51                     | 0.43              |
| 23:2O:72:VAL:O     | 23:2O:72:VAL:CG1  | 2.59                     | 0.43              |
| 25:2Q:104:GLN:HA   | 25:2Q:107:GLN:OE1 | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:2S:2:LYS:CD     | 27:2S:7:VAL:HG23   | 2.44                     | 0.43              |
| 28:2T:47:ASP:N     | 28:2T:69:LYS:O     | 2.49                     | 0.43              |
| 30:2V:12:GLN:HB3   | 30:2V:16:TRP:CZ3   | 2.54                     | 0.43              |
| 32:2X:106:VAL:O    | 32:2X:106:VAL:HG12 | 2.19                     | 0.43              |
| 47:2m:308:G:O2'    | 47:2m:309:G:OP2    | 2.28                     | 0.43              |
| 47:2m:452:G:H2'    | 47:2m:453:C:C6     | 2.54                     | 0.43              |
| 47:2m:964:A:H1'    | 47:2m:1054:G:O2'   | 2.18                     | 0.43              |
| 47:2m:1069:U:H2'   | 47:2m:1070:A:H8    | 1.84                     | 0.43              |
| 47:2m:1336:C:H2'   | 47:2m:1337:C:C6    | 2.53                     | 0.43              |
| 47:2m:1408:U:H1'   | 58:2x:71:ARG:CZ    | 2.49                     | 0.43              |
| 47:2m:1421:A:H2'   | 61:20:2:PRO:CB     | 2.36                     | 0.43              |
| 47:2m:1489:A:C6    | 50:2p:146:ARG:HD2  | 2.54                     | 0.43              |
| 48:2n:30:LEU:HD12  | 48:2n:31:ASP:H     | 1.83                     | 0.43              |
| 48:2n:111:GLN:HG2  | 48:2n:112:ILE:CD1  | 2.49                     | 0.43              |
| 49:2o:41:ILE:HG22  | 49:2o:43:ASN:O     | 2.18                     | 0.43              |
| 49:2o:174:ARG:HD3  | 49:2o:174:ARG:C    | 2.44                     | 0.43              |
| 50:2p:17:PHE:CD2   | 50:2p:18:LYS:HG2   | 2.53                     | 0.43              |
| 50:2p:194:PRO:HA   | 50:2p:201:LYS:HG3  | 2.01                     | 0.43              |
| 52:2r:127:ARG:HD2  | 52:2r:127:ARG:HA   | 1.85                     | 0.43              |
| 53:2s:122:LEU:HD21 | 53:2s:126:HIS:CE1  | 2.54                     | 0.43              |
| 54:2t:148:LYS:C    | 54:2t:151:GLU:HG3  | 2.43                     | 0.43              |
| 56:2v:30:LYS:CG    | 56:2v:31:GLU:N     | 2.82                     | 0.43              |
| 57:2w:100:LYS:CG   | 57:2w:101:THR:HG22 | 2.49                     | 0.43              |
| 60:2z:13:LEU:HD21  | 60:2z:15:VAL:HG22  | 2.00                     | 0.43              |
| 60:2z:120:HIS:CE1  | 60:2z:124:ARG:HD2  | 2.54                     | 0.43              |
| 62:21:46:LYS:HG3   | 62:21:46:LYS:O     | 2.18                     | 0.43              |
| 63:3A:39:VAL:HA    | 63:3A:45:ARG:O     | 2.18                     | 0.43              |
| 63:3A:74:LYS:NZ    | 63:3A:83:PHE:HD1   | 2.17                     | 0.43              |
| 68:3F:158:PRO:HG3  | 68:3F:200:VAL:HG23 | 2.01                     | 0.43              |
| 68:3F:168:CYS:HB2  | 68:3F:195:LEU:CB   | 2.49                     | 0.43              |
| 71:3I:53:ILE:HD13  | 71:3I:81:LEU:HD21  | 2.01                     | 0.43              |
| 1:1A:189:G:C2      | 1:1A:253:G:N1      | 2.87                     | 0.43              |
| 1:1A:965:G:O2'     | 1:1A:966:A:H5''    | 2.18                     | 0.43              |
| 1:1A:1447:C:O2     | 1:1A:1447:C:H2'    | 2.17                     | 0.43              |
| 1:1A:1541:C:H2'    | 1:1A:1542:U:C6     | 2.54                     | 0.43              |
| 1:1A:1669:A:H2'    | 1:1A:1670:G:O4'    | 2.19                     | 0.43              |
| 1:1A:1671:U:O4     | 1:1A:1853:G:H1'    | 2.19                     | 0.43              |
| 1:1A:3976:C:O2'    | 1:1A:3977:C:O4'    | 2.35                     | 0.43              |
| 1:1A:4129:G:O2'    | 1:1A:4130:C:H5'    | 2.19                     | 0.43              |
| 1:1A:4396:A:O2'    | 1:1A:4397:A:H5'    | 2.19                     | 0.43              |
| 1:1A:4598:C:H2'    | 1:1A:4611:A:H61    | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:5021:C:H2'    | 1:1A:5022:U:C4'    | 2.49                     | 0.43              |
| 4:1D:86:GLN:HG2    | 4:1D:87:PHE:N      | 2.34                     | 0.43              |
| 4:1D:247:ARG:HB3   | 4:1D:247:ARG:CZ    | 2.48                     | 0.43              |
| 11:2C:54:ARG:HH11  | 11:2C:54:ARG:HG3   | 1.84                     | 0.43              |
| 11:2C:173:ARG:O    | 11:2C:176:LEU:HD21 | 2.19                     | 0.43              |
| 15:2G:122:ILE:HD12 | 17:2I:189:ILE:HG22 | 2.00                     | 0.43              |
| 21:2M:30:MET:HE1   | 21:2M:47:PHE:CB    | 2.49                     | 0.43              |
| 30:2V:98:TYR:CE1   | 30:2V:104:LEU:HB3  | 2.54                     | 0.43              |
| 34:2Z:41:PHE:CZ    | 34:2Z:105:LEU:HD13 | 2.54                     | 0.43              |
| 36:2b:82:ASP:OD1   | 36:2b:82:ASP:N     | 2.45                     | 0.43              |
| 46:2l:17:VAL:O     | 46:2l:18:LEU:C     | 2.62                     | 0.43              |
| 47:2m:309:G:H2'    | 47:2m:310:C:O4'    | 2.19                     | 0.43              |
| 47:2m:574:A:HO2'   | 47:2m:575:A:H8     | 1.59                     | 0.43              |
| 47:2m:837:A:N6     | 76:3N:9:THR:HG22   | 2.34                     | 0.43              |
| 47:2m:883:U:H6     | 47:2m:883:U:H3'    | 1.84                     | 0.43              |
| 47:2m:915:G:OP2    | 47:2m:915:G:N2     | 2.47                     | 0.43              |
| 47:2m:1325:G:H1'   | 47:2m:1510:G:H5''  | 2.01                     | 0.43              |
| 48:2n:36:GLN:O     | 48:2n:53:ARG:NH2   | 2.51                     | 0.43              |
| 48:2n:49:ILE:HG21  | 48:2n:162:PRO:O    | 2.18                     | 0.43              |
| 48:2n:168:ALA:HB1  | 48:2n:204:TYR:HB3  | 1.99                     | 0.43              |
| 49:2o:82:ARG:NH2   | 49:2o:191:ASP:HB2  | 2.33                     | 0.43              |
| 50:2p:59:LEU:HD21  | 50:2p:66:ILE:HD12  | 2.01                     | 0.43              |
| 52:2r:20:PHE:HD1   | 52:2r:20:PHE:O     | 2.02                     | 0.43              |
| 52:2r:26:ASP:OD1   | 52:2r:43:GLU:HB3   | 2.18                     | 0.43              |
| 52:2r:49:LEU:CG    | 58:2x:49:TYR:HB2   | 2.49                     | 0.43              |
| 52:2r:75:SER:O     | 52:2r:78:MET:HG2   | 2.19                     | 0.43              |
| 57:2w:56:LEU:O     | 57:2w:60:LEU:HD22  | 2.19                     | 0.43              |
| 57:2w:93:MET:HE3   | 57:2w:104:GLN:NE2  | 2.34                     | 0.43              |
| 61:20:60:THR:O     | 61:20:64:LEU:HD23  | 2.19                     | 0.43              |
| 62:21:21:ARG:NH1   | 62:21:90:ASP:OD2   | 2.51                     | 0.43              |
| 71:3I:114:VAL:HG13 | 71:3I:119:LEU:CB   | 2.49                     | 0.43              |
| 72:3J:113:ASP:OD1  | 72:3J:113:ASP:N    | 2.51                     | 0.43              |
| 75:3M:74:VAL:HG23  | 75:3M:126:LEU:O    | 2.19                     | 0.43              |
| 77:3O:63:PRO:CA    | 77:3O:97:ILE:HD11  | 2.48                     | 0.43              |
| 1:1A:122:U:H1'     | 1:1A:152:U:O2      | 2.19                     | 0.42              |
| 1:1A:186:G:H4'     | 1:1A:187:U:O4'     | 2.19                     | 0.42              |
| 1:1A:418:A:O2'     | 1:1A:419:A:H5'     | 2.19                     | 0.42              |
| 1:1A:685:C:O5'     | 1:1A:685:C:H6      | 2.02                     | 0.42              |
| 1:1A:1076:C:H2'    | 1:1A:1077:C:C6     | 2.53                     | 0.42              |
| 1:1A:1367:C:O2     | 1:1A:1367:C:O4'    | 2.37                     | 0.42              |
| 1:1A:1383:G:H2'    | 1:1A:1384:C:C6     | 2.54                     | 0.42              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 1:1A:2352:U:H2'      | 1:1A:2353:U:C6     | 2.54                     | 0.42              |
| 1:1A:2830:G:C6       | 1:1A:3856:A:N6     | 2.87                     | 0.42              |
| 1:1A:4155:C:C2'      | 1:1A:4156:G:H5'    | 2.49                     | 0.42              |
| 1:1A:4229:U:O2       | 1:1A:4229:U:H2'    | 2.18                     | 0.42              |
| 1:1A:4428:A:O2'      | 1:1A:4429:C:H5'    | 2.19                     | 0.42              |
| 1:1A:4475:G:OP2      | 11:2C:173:ARG:NH2  | 2.52                     | 0.42              |
| 1:1A:4762:A:H2       | 21:2M:173:ASN:HA   | 1.83                     | 0.42              |
| 2:1B:5:A:O2'         | 2:1B:6:C:H5'       | 2.19                     | 0.42              |
| 5:1E:17:LEU:HB3      | 5:1E:18:PRO:CD     | 2.46                     | 0.42              |
| 6:1F:64:ALA:HB1      | 6:1F:78:ARG:O      | 2.19                     | 0.42              |
| 6:1F:367:GLU:O       | 6:1F:368:LYS:HG2   | 2.19                     | 0.42              |
| 7:1G:41:LYS:HD3      | 7:1G:41:LYS:HA     | 1.62                     | 0.42              |
| 10:2B:137[B]:ARG:HD2 | 10:2B:205:THR:HG21 | 2.00                     | 0.42              |
| 13:2E:48:PRO:HB2     | 13:2E:70:VAL:HG22  | 2.00                     | 0.42              |
| 16:2H:148:THR:O      | 16:2H:151:ILE:HG22 | 2.19                     | 0.42              |
| 23:2O:44:GLN:HB2     | 23:2O:63:ILE:HD11  | 2.01                     | 0.42              |
| 24:2P:99:GLU:HG3     | 25:2Q:21:TYR:HH    | 1.82                     | 0.42              |
| 25:2Q:101:ARG:HB3    | 25:2Q:101:ARG:CZ   | 2.49                     | 0.42              |
| 30:2V:102:PRO:C      | 30:2V:109:ARG:HH22 | 2.24                     | 0.42              |
| 32:2X:27:ILE:HG22    | 32:2X:29:ILE:HD13  | 2.01                     | 0.42              |
| 32:2X:46:LEU:HD12    | 32:2X:64:ILE:HD13  | 2.01                     | 0.42              |
| 33:2Y:86:GLU:OE2     | 33:2Y:114:ARG:NE   | 2.52                     | 0.42              |
| 41:2g:99:CYS:HB2     | 41:2g:114:LYS:HD2  | 2.01                     | 0.42              |
| 42:2h:8:LYS:HE2      | 47:2m:1847:G:O6    | 2.19                     | 0.42              |
| 46:2l:180:VAL:HG23   | 46:2l:181:TYR:H    | 1.84                     | 0.42              |
| 47:2m:306:C:H2'      | 47:2m:307:G:C2     | 2.54                     | 0.42              |
| 47:2m:449:A:O2'      | 47:2m:450:C:H4'    | 2.18                     | 0.42              |
| 47:2m:692:G:H4'      | 47:2m:692:G:OP1    | 2.18                     | 0.42              |
| 47:2m:824:C:C2'      | 47:2m:825:A:H5'    | 2.49                     | 0.42              |
| 47:2m:943:U:C2       | 47:2m:944:A:C8     | 3.07                     | 0.42              |
| 47:2m:1219:C:H4'     | 66:3D:24:GLN:HG2   | 2.01                     | 0.42              |
| 47:2m:1291:A:H62     | 47:2m:1302:G:N2    | 2.18                     | 0.42              |
| 47:2m:1294:G:P       | 47:2m:1294:G:H8    | 2.42                     | 0.42              |
| 47:2m:1837:G:H5''    | 47:2m:1838:U:O5'   | 2.19                     | 0.42              |
| 48:2n:65:ILE:HG21    | 48:2n:182:VAL:HG22 | 2.01                     | 0.42              |
| 49:2o:138:PHE:O      | 49:2o:213:ARG:N    | 2.52                     | 0.42              |
| 50:2p:49:ILE:HA      | 50:2p:87:TYR:HB2   | 2.00                     | 0.42              |
| 50:2p:69:LEU:HA      | 50:2p:72:VAL:CG2   | 2.49                     | 0.42              |
| 50:2p:123:LEU:HD13   | 50:2p:127:MET:SD   | 2.59                     | 0.42              |
| 50:2p:162:ASP:O      | 50:2p:163:PRO:C    | 2.62                     | 0.42              |
| 51:2q:71:LYS:NZ      | 51:2q:74:GLY:HA2   | 2.33                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:2q:97:GLU:HB3   | 51:2q:99:PHE:CZ    | 2.54                     | 0.42              |
| 52:2r:82:ASN:OD1   | 52:2r:82:ASN:N     | 2.51                     | 0.42              |
| 53:2s:69:LEU:O     | 53:2s:73:GLN:HG3   | 2.19                     | 0.42              |
| 58:2x:53:GLU:OE1   | 58:2x:85:ARG:HD2   | 2.19                     | 0.42              |
| 59:2y:17:ILE:HD13  | 59:2y:17:ILE:N     | 2.34                     | 0.42              |
| 59:2y:34:VAL:HA    | 59:2y:37:GLU:OE2   | 2.18                     | 0.42              |
| 60:2z:120:HIS:HE1  | 60:2z:124:ARG:HH11 | 1.65                     | 0.42              |
| 61:20:38:LYS:HD3   | 61:20:41:LYS:CA    | 2.48                     | 0.42              |
| 70:3H:147:LEU:HD11 | 70:3H:156:TYR:CD2  | 2.53                     | 0.42              |
| 71:3I:130:ILE:O    | 71:3I:143:ASN:HA   | 2.19                     | 0.42              |
| 73:3K:98:VAL:CG1   | 73:3K:115:LEU:HB2  | 2.49                     | 0.42              |
| 75:3M:57:ARG:HD2   | 75:3M:57:ARG:N     | 2.31                     | 0.42              |
| 78:3P:35:VAL:CG1   | 78:3P:46:VAL:HG23  | 2.48                     | 0.42              |
| 78:3P:56:CYS:CB    | 78:3P:59:CYS:HB3   | 2.48                     | 0.42              |
| 1:1A:93:G:O2'      | 1:1A:94:A:H5'      | 2.19                     | 0.42              |
| 1:1A:360:A:C4      | 3:1C:24:G:H1'      | 2.54                     | 0.42              |
| 1:1A:1247:U:O2'    | 1:1A:1248:C:H5'    | 2.20                     | 0.42              |
| 1:1A:1720:C:H2'    | 1:1A:1721:G:C8     | 2.54                     | 0.42              |
| 1:1A:1914:C:H4'    | 17:2I:89:PRO:HD3   | 2.02                     | 0.42              |
| 1:1A:2481:G:N2     | 1:1A:2498:C:H41    | 2.17                     | 0.42              |
| 1:1A:3693:U:O3'    | 44:2j:21:SER:HB2   | 2.19                     | 0.42              |
| 1:1A:3952:A:H2     | 1:1A:4056:A:C2     | 2.37                     | 0.42              |
| 1:1A:4075:U:OP1    | 10:2B:246:SER:OG   | 2.33                     | 0.42              |
| 1:1A:4237:C:OP1    | 1:1A:4327:C:O2'    | 2.34                     | 0.42              |
| 4:1D:83:HIS:HB3    | 44:2j:64:VAL:HG22  | 2.01                     | 0.42              |
| 11:2C:63:ASN:O     | 11:2C:67:LEU:HG    | 2.19                     | 0.42              |
| 12:2D:156:LYS:HG2  | 12:2D:163:GLN:HB2  | 2.01                     | 0.42              |
| 13:2E:9:GLU:HB2    | 13:2E:13:ARG:CB    | 2.49                     | 0.42              |
| 19:2K:133:GLY:O    | 19:2K:136:THR:OG1  | 2.34                     | 0.42              |
| 25:2Q:64:SER:C     | 25:2Q:65:GLU:HG3   | 2.44                     | 0.42              |
| 30:2V:5:LYS:HE3    | 30:2V:8:THR:HB     | 2.02                     | 0.42              |
| 35:2a:85:LYS:HB2   | 35:2a:85:LYS:HE2   | 1.82                     | 0.42              |
| 46:2l:198:TRP:CG   | 46:2l:199:GLN:N    | 2.87                     | 0.42              |
| 47:2m:550:C:C6     | 47:2m:550:C:OP2    | 2.72                     | 0.42              |
| 47:2m:850:C:HO2'   | 47:2m:851:C:P      | 2.40                     | 0.42              |
| 47:2m:1263:U:H3'   | 47:2m:1264:C:C6    | 2.54                     | 0.42              |
| 47:2m:1588:A:H3'   | 47:2m:1588:A:P     | 2.59                     | 0.42              |
| 47:2m:1607:A:H2'   | 47:2m:1608:U:H6    | 1.83                     | 0.42              |
| 47:2m:1740:C:O2'   | 47:2m:1741:U:H5'   | 2.19                     | 0.42              |
| 47:2m:1809:A:H2'   | 47:2m:1810:U:C6    | 2.54                     | 0.42              |
| 49:2o:171:ILE:CD1  | 49:2o:197:ILE:HD13 | 2.48                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:2p:68:GLU:HG3   | 55:2u:70:TYR:HE2   | 1.84                     | 0.42              |
| 51:2q:122:LYS:CD   | 51:2q:162:ILE:HD11 | 2.50                     | 0.42              |
| 52:2r:188:TYR:CD1  | 52:2r:188:TYR:C    | 2.97                     | 0.42              |
| 53:2s:98:ARG:CB    | 53:2s:125:VAL:HG22 | 2.40                     | 0.42              |
| 58:2x:25:CYS:SG    | 58:2x:68:ILE:HD12  | 2.60                     | 0.42              |
| 59:2y:104:GLU:OE1  | 59:2y:104:GLU:HA   | 2.19                     | 0.42              |
| 64:3B:84:PHE:HE2   | 64:3B:86:PRO:HB3   | 1.84                     | 0.42              |
| 68:3F:104:HIS:CE1  | 68:3F:130:LYS:HG3  | 2.54                     | 0.42              |
| 68:3F:152:SER:O    | 68:3F:154:VAL:HG23 | 2.18                     | 0.42              |
| 69:3G:137:VAL:O    | 69:3G:162:ILE:HA   | 2.18                     | 0.42              |
| 69:3G:213:LEU:HD21 | 69:3G:240:THR:CG2  | 2.48                     | 0.42              |
| 80:3R:119:ARG:HH22 | 80:3R:148:TYR:HE2  | 1.67                     | 0.42              |
| 1:1A:302:C:H2'     | 1:1A:303:C:C6      | 2.55                     | 0.42              |
| 1:1A:1186:U:H3'    | 1:1A:1187:G:N2     | 2.35                     | 0.42              |
| 1:1A:1664:U:H2'    | 1:1A:1665:C:H6     | 1.84                     | 0.42              |
| 1:1A:1806:G:H2'    | 1:1A:1807:C:C6     | 2.54                     | 0.42              |
| 1:1A:1874:A:H2'    | 1:1A:1875:C:C6     | 2.54                     | 0.42              |
| 1:1A:2029:A:H2'    | 1:1A:2030:A:C8     | 2.54                     | 0.42              |
| 1:1A:2389:A:C2'    | 1:1A:2390:G:O5'    | 2.67                     | 0.42              |
| 1:1A:2485:U:OP1    | 1:1A:2486:G:N2     | 2.33                     | 0.42              |
| 1:1A:2497:C:H2'    | 1:1A:2498:C:C6     | 2.54                     | 0.42              |
| 1:1A:2607:C:H2'    | 1:1A:2608:G:C8     | 2.54                     | 0.42              |
| 1:1A:2728:U:H2'    | 1:1A:2729:C:H6     | 1.84                     | 0.42              |
| 1:1A:2835:A:C1'    | 1:1A:4979:A:H5'    | 2.48                     | 0.42              |
| 1:1A:2835:A:O4'    | 1:1A:4979:A:H5'    | 2.19                     | 0.42              |
| 1:1A:2856:C:O2     | 1:1A:2856:C:H2'    | 2.19                     | 0.42              |
| 1:1A:2893:U:H2'    | 1:1A:2894:A:C8     | 2.54                     | 0.42              |
| 1:1A:4407:G:H1'    | 1:1A:4438:U:C2     | 2.54                     | 0.42              |
| 1:1A:4618:G:H5''   | 24:2P:15:ARG:HB2   | 2.01                     | 0.42              |
| 1:1A:4653:C:H2'    | 1:1A:4654:C:C6     | 2.54                     | 0.42              |
| 1:1A:4678:G:N2     | 1:1A:4713:G:C1'    | 2.75                     | 0.42              |
| 6:1F:143:ARG:HG2   | 6:1F:182:LYS:HD2   | 2.01                     | 0.42              |
| 7:1G:234:ASP:C     | 7:1G:236:MET:H     | 2.28                     | 0.42              |
| 13:2E:14:GLU:HG2   | 13:2E:137:PRO:HG2  | 2.02                     | 0.42              |
| 14:2F:96:ILE:O     | 14:2F:96:ILE:HG22  | 2.18                     | 0.42              |
| 21:2M:44:PHE:CD2   | 21:2M:61:ILE:HD11  | 2.54                     | 0.42              |
| 23:2O:28:PRO:HB2   | 23:2O:34:MET:HB3   | 2.01                     | 0.42              |
| 23:2O:66:SER:C     | 23:2O:68:SER:H     | 2.27                     | 0.42              |
| 23:2O:76:VAL:C     | 23:2O:78:PHE:H     | 2.27                     | 0.42              |
| 33:2Y:72:SER:O     | 33:2Y:74:PHE:N     | 2.52                     | 0.42              |
| 35:2a:24:ARG:HB2   | 35:2a:30:ILE:HD13  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:189:U:O3'    | 47:2m:190:G:O4'    | 2.37                     | 0.42              |
| 47:2m:545:A:H2'    | 47:2m:547:G:N2     | 2.33                     | 0.42              |
| 47:2m:587:A:H5''   | 47:2m:592:C:H5     | 1.82                     | 0.42              |
| 47:2m:659:G:H2'    | 47:2m:663:C:C5     | 2.53                     | 0.42              |
| 47:2m:1036:A:H4'   | 47:2m:1855:G:H21   | 1.84                     | 0.42              |
| 47:2m:1076:G:OP1   | 73:3K:106:ARG:NH2  | 2.52                     | 0.42              |
| 47:2m:1236:G:O2'   | 47:2m:1237:C:H5'   | 2.19                     | 0.42              |
| 47:2m:1243:U:OP2   | 47:2m:1518:C:H1'   | 2.19                     | 0.42              |
| 47:2m:1338:G:O3'   | 62:21:74:SER:OG    | 2.21                     | 0.42              |
| 47:2m:1650:A:H5''  | 58:2x:139:ALA:HB2  | 2.01                     | 0.42              |
| 48:2n:77:ILE:HD11  | 48:2n:99:ILE:HD12  | 2.01                     | 0.42              |
| 49:2o:69:VAL:CG1   | 49:2o:74:LEU:HD11  | 2.42                     | 0.42              |
| 50:2p:176:LEU:CD1  | 50:2p:181:VAL:HG12 | 2.49                     | 0.42              |
| 51:2q:61:VAL:O     | 51:2q:64:ILE:HG12  | 2.19                     | 0.42              |
| 51:2q:72:ILE:CD1   | 51:2q:77:ARG:HB2   | 2.50                     | 0.42              |
| 51:2q:164:LEU:O    | 51:2q:165:GLU:HB3  | 2.19                     | 0.42              |
| 51:2q:167:GLY:C    | 51:2q:168:LYS:HD3  | 2.43                     | 0.42              |
| 53:2s:62:ILE:HG21  | 53:2s:94:PHE:CE2   | 2.54                     | 0.42              |
| 53:2s:132:ASP:OD1  | 53:2s:133:LEU:N    | 2.53                     | 0.42              |
| 56:2v:22:ARG:C     | 56:2v:22:ARG:CD    | 2.93                     | 0.42              |
| 58:2x:15:ARG:HG3   | 58:2x:15:ARG:HH11  | 1.85                     | 0.42              |
| 58:2x:39:LEU:CG    | 58:2x:51:LEU:HD21  | 2.49                     | 0.42              |
| 61:20:112:MET:O    | 61:20:123:LEU:HD22 | 2.19                     | 0.42              |
| 62:21:61:LEU:HD13  | 62:21:82:MET:CE    | 2.49                     | 0.42              |
| 68:3F:261:LEU:HD12 | 68:3F:261:LEU:HA   | 1.85                     | 0.42              |
| 70:3H:121:ILE:HG22 | 70:3H:124:LEU:CB   | 2.49                     | 0.42              |
| 71:3I:36:GLY:O     | 71:3I:127:ARG:HD2  | 2.19                     | 0.42              |
| 77:3O:47:LEU:HD13  | 77:3O:79:ILE:HD12  | 2.01                     | 0.42              |
| 1:1A:139:G:C3'     | 1:1A:140:G:C8      | 3.02                     | 0.42              |
| 1:1A:216:C:H5'     | 1:1A:219:G:N2      | 2.34                     | 0.42              |
| 1:1A:1285:U:O2'    | 1:1A:1286:C:H5'    | 2.19                     | 0.42              |
| 1:1A:1554:A:OP2    | 44:2j:4:ARG:NE     | 2.50                     | 0.42              |
| 1:1A:1664:U:H2'    | 1:1A:1665:C:C6     | 2.54                     | 0.42              |
| 1:1A:1837:A:OP2    | 22:2N:130:ARG:HG2  | 2.20                     | 0.42              |
| 1:1A:2832:A:O2'    | 1:1A:2833:A:H5'    | 2.19                     | 0.42              |
| 1:1A:4183:G:H2'    | 1:1A:4183:G:N3     | 2.34                     | 0.42              |
| 1:1A:4239:A:O2'    | 1:1A:4240:G:H5'    | 2.18                     | 0.42              |
| 1:1A:4650:G:C2'    | 1:1A:4651:A:H5'    | 2.50                     | 0.42              |
| 1:1A:4743:G:H22    | 1:1A:4956:A:H2     | 1.67                     | 0.42              |
| 5:1E:4:ARG:O       | 5:1E:5:LYS:HG2     | 2.19                     | 0.42              |
| 5:1E:133:TYR:O     | 5:1E:136:LYS:HG2   | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:2D:7:ARG:NH1    | 12:2D:7:ARG:HB2    | 2.34                     | 0.42              |
| 12:2D:42:LYS:HD3   | 12:2D:42:LYS:HA    | 1.68                     | 0.42              |
| 13:2E:9:GLU:O      | 13:2E:13:ARG:HB2   | 2.20                     | 0.42              |
| 13:2E:93:GLU:HG2   | 13:2E:173:ILE:HG13 | 2.01                     | 0.42              |
| 14:2F:80:GLU:OE2   | 14:2F:113:ASN:ND2  | 2.51                     | 0.42              |
| 14:2F:200:LYS:NZ   | 14:2F:200:LYS:HB2  | 2.32                     | 0.42              |
| 19:2K:49:LYS:HG2   | 19:2K:53:MET:HE3   | 2.02                     | 0.42              |
| 31:2W:36:LYS:HE2   | 31:2W:36:LYS:HB3   | 1.53                     | 0.42              |
| 38:2d:21:ARG:O     | 38:2d:22:CYS:SG    | 2.77                     | 0.42              |
| 45:2k:105:ASP:OD1  | 45:2k:105:ASP:N    | 2.51                     | 0.42              |
| 46:2l:23:ARG:NH1   | 46:2l:176:ASP:OD2  | 2.53                     | 0.42              |
| 46:2l:179:LEU:CA   | 46:2l:182:ASN:HB3  | 2.38                     | 0.42              |
| 47:2m:27:A:N1      | 47:2m:647:U:H5     | 2.17                     | 0.42              |
| 47:2m:38:A:OP1     | 71:3l:5:ARG:HG3    | 2.19                     | 0.42              |
| 47:2m:118:C:H1'    | 47:2m:445:A:N7     | 2.33                     | 0.42              |
| 47:2m:162:C:H2'    | 47:2m:163:U:O4'    | 2.18                     | 0.42              |
| 47:2m:377:G:H5'    | 54:2t:98:LYS:CB    | 2.28                     | 0.42              |
| 47:2m:548:C:N3     | 47:2m:549:C:N4     | 2.66                     | 0.42              |
| 47:2m:558:G:C4     | 47:2m:559:G:N2     | 2.79                     | 0.42              |
| 47:2m:731:G:OP1    | 47:2m:732:U:H4'    | 2.19                     | 0.42              |
| 47:2m:751:G:O6     | 47:2m:753:C:H5'    | 2.20                     | 0.42              |
| 47:2m:1099:G:H22   | 47:2m:1133:A:H2    | 1.68                     | 0.42              |
| 47:2m:1203:G:N2    | 47:2m:1699:A:H8    | 2.02                     | 0.42              |
| 47:2m:1276:A:H3'   | 47:2m:1277:C:C6    | 2.54                     | 0.42              |
| 47:2m:1288:U:H2'   | 47:2m:1289:U:C5    | 2.54                     | 0.42              |
| 47:2m:1324:G:H2'   | 47:2m:1325:G:O4'   | 2.18                     | 0.42              |
| 47:2m:1487:A:O2'   | 47:2m:1488:C:H5'   | 2.19                     | 0.42              |
| 47:2m:1657:G:O2'   | 47:2m:1658:G:H5'   | 2.20                     | 0.42              |
| 47:2m:1677:U:H5''  | 52:2r:148:ASN:HD22 | 1.83                     | 0.42              |
| 47:2m:1860:A:OP1   | 65:3C:8:ASN:CB     | 2.67                     | 0.42              |
| 50:2p:105:LEU:HD12 | 50:2p:105:LEU:O    | 2.20                     | 0.42              |
| 52:2r:76:MET:HE3   | 52:2r:76:MET:O     | 2.19                     | 0.42              |
| 52:2r:162:ALA:HB2  | 52:2r:172:CYS:SG   | 2.59                     | 0.42              |
| 53:2s:7:LYS:HE2    | 53:2s:10:LYS:HZ3   | 1.84                     | 0.42              |
| 53:2s:95:ILE:HG23  | 53:2s:132:ASP:OD2  | 2.19                     | 0.42              |
| 53:2s:134:VAL:O    | 53:2s:134:VAL:HG23 | 2.19                     | 0.42              |
| 54:2t:37:LYS:O     | 54:2t:59:ARG:HA    | 2.19                     | 0.42              |
| 55:2u:41:PRO:O     | 55:2u:45:VAL:HG13  | 2.19                     | 0.42              |
| 58:2x:123:ASP:OD1  | 58:2x:124:PRO:HD2  | 2.20                     | 0.42              |
| 60:2z:80:PRO:HG2   | 60:2z:83:PHE:CE2   | 2.53                     | 0.42              |
| 61:20:10:ASN:HB3   | 61:20:13:GLU:HB3   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:20:64:LEU:CD2   | 61:20:75:MET:HE2   | 2.49                     | 0.42              |
| 63:3A:39:VAL:HB    | 63:3A:44:GLY:C     | 2.44                     | 0.42              |
| 68:3F:68:ASP:OD2   | 68:3F:111:VAL:HG22 | 2.19                     | 0.42              |
| 68:3F:225:LYS:HB2  | 68:3F:225:LYS:HE3  | 1.61                     | 0.42              |
| 70:3H:222:GLU:HA   | 70:3H:225:GLN:HG2  | 2.00                     | 0.42              |
| 1:1A:206:U:O2'     | 1:1A:208:A:N7      | 2.40                     | 0.42              |
| 1:1A:1326:A:C2     | 1:1A:1327:C:C4     | 3.08                     | 0.42              |
| 1:1A:1520:C:O2'    | 1:1A:1521:C:H5'    | 2.20                     | 0.42              |
| 1:1A:2256:C:H2'    | 1:1A:2257:C:C6     | 2.44                     | 0.42              |
| 1:1A:2676:A:C4     | 1:1A:2677:G:C8     | 3.07                     | 0.42              |
| 1:1A:3611:A:O2'    | 1:1A:5016:A:O2'    | 2.16                     | 0.42              |
| 1:1A:3652:A:C2'    | 1:1A:3653:A:C8     | 3.02                     | 0.42              |
| 1:1A:3692:A:H62    | 1:1A:3823:G:H21    | 0.66                     | 0.42              |
| 1:1A:4064:C:H2'    | 1:1A:4065:G:O4'    | 2.18                     | 0.42              |
| 1:1A:4525:C:O2'    | 1:1A:4526:U:H5'    | 2.19                     | 0.42              |
| 1:1A:4717:A:OP2    | 5:1E:30:LYS:NZ     | 2.35                     | 0.42              |
| 1:1A:4910:G:H4'    | 5:1E:95:THR:CG2    | 2.48                     | 0.42              |
| 1:1A:4931:G:H2'    | 1:1A:4931:G:N3     | 2.33                     | 0.42              |
| 1:1A:5055:G:H2'    | 1:1A:5056:A:C8     | 2.54                     | 0.42              |
| 3:1C:89:U:H2'      | 3:1C:90:C:H6       | 1.81                     | 0.42              |
| 5:1E:305:THR:O     | 5:1E:305:THR:HG23  | 2.19                     | 0.42              |
| 8:1H:164:PHE:HE1   | 8:1H:173:LEU:HB3   | 1.84                     | 0.42              |
| 11:2C:50:LYS:HD2   | 11:2C:50:LYS:N     | 2.34                     | 0.42              |
| 14:2F:58:ILE:HG12  | 14:2F:116:ARG:HD2  | 2.00                     | 0.42              |
| 18:2J:41:ILE:HG23  | 18:2J:42:ARG:N     | 2.34                     | 0.42              |
| 18:2J:94:MET:HE3   | 18:2J:94:MET:HB2   | 1.71                     | 0.42              |
| 24:2P:120:PRO:HA   | 24:2P:138:SER:O    | 2.19                     | 0.42              |
| 37:2c:77:VAL:HG23  | 37:2c:78:GLY:N     | 2.35                     | 0.42              |
| 41:2g:79:GLU:HG3   | 41:2g:82:LEU:H     | 1.83                     | 0.42              |
| 46:2l:32:VAL:HG23  | 46:2l:206:ILE:HG13 | 2.00                     | 0.42              |
| 46:2l:38:LEU:C     | 46:2l:38:LEU:HD13  | 2.45                     | 0.42              |
| 46:2l:148:VAL:HG22 | 46:2l:149:ASP:N    | 2.33                     | 0.42              |
| 47:2m:635:G:H4'    | 79:3Q:19:VAL:HG12  | 2.02                     | 0.42              |
| 47:2m:1013:U:OP1   | 47:2m:1129:G:O2'   | 2.37                     | 0.42              |
| 47:2m:1018:U:H4'   | 73:3K:47:PRO:HB2   | 2.01                     | 0.42              |
| 47:2m:1174:U:H2'   | 47:2m:1175:G:H8    | 1.85                     | 0.42              |
| 47:2m:1386:A:OP2   | 50:2p:160:SER:OG   | 2.38                     | 0.42              |
| 47:2m:1462:U:H2'   | 47:2m:1464:C:H42   | 1.83                     | 0.42              |
| 47:2m:1511:U:O2'   | 47:2m:1512:C:C6    | 2.67                     | 0.42              |
| 47:2m:1529:C:H2'   | 47:2m:1530:U:C6    | 2.54                     | 0.42              |
| 47:2m:1649:U:OP1   | 58:2x:128:GLU:HB2  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1787:G:O2'   | 47:2m:1788:A:H5'   | 2.20                     | 0.42              |
| 48:2n:103:PHE:CE1  | 48:2n:107:THR:HB   | 2.54                     | 0.42              |
| 48:2n:140:VAL:C    | 48:2n:141:ASN:OD1  | 2.62                     | 0.42              |
| 48:2n:170:SER:O    | 48:2n:174:MET:CE   | 2.66                     | 0.42              |
| 50:2p:74:GLN:NE2   | 50:2p:81:GLU:OE2   | 2.52                     | 0.42              |
| 51:2q:159:THR:OG1  | 51:2q:227:VAL:HB   | 2.20                     | 0.42              |
| 52:2r:33:ILE:HA    | 52:2r:36:GLN:HG2   | 2.02                     | 0.42              |
| 53:2s:147:LYS:HA   | 75:3M:49:GLU:OE2   | 2.19                     | 0.42              |
| 59:2y:58:MET:HA    | 59:2y:61:ILE:CG1   | 2.50                     | 0.42              |
| 59:2y:81:ARG:HD2   | 59:2y:82:ASP:N     | 2.33                     | 0.42              |
| 60:2z:23:ARG:NH2   | 77:3O:45:ASN:OD1   | 2.52                     | 0.42              |
| 60:2z:61:GLU:HA    | 60:2z:64:VAL:HG12  | 2.02                     | 0.42              |
| 64:3B:107:ARG:CD   | 64:3B:112:VAL:HG22 | 2.50                     | 0.42              |
| 68:3F:81:GLY:N     | 68:3F:87:LEU:HD23  | 2.34                     | 0.42              |
| 70:3H:20:ASP:OD2   | 70:3H:22:ARG:HB2   | 2.18                     | 0.42              |
| 71:3I:142:VAL:HG11 | 71:3I:147:PHE:CD2  | 2.54                     | 0.42              |
| 75:3M:57:ARG:NH2   | 78:3P:26:GLN:OE1   | 2.53                     | 0.42              |
| 75:3M:104:LEU:HD12 | 75:3M:106:THR:CG2  | 2.50                     | 0.42              |
| 1:1A:62:A:OP1      | 16:2H:172:ARG:NH1  | 2.47                     | 0.42              |
| 1:1A:128:C:H2'     | 1:1A:129:C:N1      | 2.34                     | 0.42              |
| 1:1A:274:C:C2'     | 1:1A:275:C:H5'     | 2.49                     | 0.42              |
| 1:1A:510:U:H5'     | 29:2U:86:THR:OG1   | 2.19                     | 0.42              |
| 1:1A:1301:C:H42    | 33:2Y:14:LYS:CG    | 2.32                     | 0.42              |
| 1:1A:1763:C:H2'    | 1:1A:1764:G:C5'    | 2.38                     | 0.42              |
| 1:1A:1767:A:H62    | 57:2w:10:ARG:CG    | 2.33                     | 0.42              |
| 1:1A:2395:A:H5'    | 1:1A:2397:G:O4'    | 2.19                     | 0.42              |
| 1:1A:2768:C:H4'    | 1:1A:2769:U:OP2    | 2.20                     | 0.42              |
| 1:1A:2853:C:H2'    | 1:1A:2854:G:O4'    | 2.18                     | 0.42              |
| 1:1A:3789:C:H2'    | 1:1A:3790:U:C5     | 2.55                     | 0.42              |
| 1:1A:3888:G:HO2'   | 1:1A:3889:G:P      | 2.43                     | 0.42              |
| 1:1A:3951:G:H2'    | 1:1A:3952:A:O5'    | 2.20                     | 0.42              |
| 1:1A:4098:A:O2'    | 1:1A:4099:G:OP1    | 2.31                     | 0.42              |
| 1:1A:4257:A:H2     | 13:2E:27:GLY:O     | 2.02                     | 0.42              |
| 1:1A:4347:G:C6     | 1:1A:4366:A:C6     | 3.08                     | 0.42              |
| 1:1A:4466:C:C2     | 1:1A:4467:A:C8     | 3.08                     | 0.42              |
| 1:1A:4517:A:O2'    | 5:1E:258:HIS:HB2   | 2.20                     | 0.42              |
| 1:1A:4767:C:C2'    | 1:1A:4874:A:H62    | 2.31                     | 0.42              |
| 1:1A:4945:G:O6     | 34:2Z:4:ARG:O      | 2.37                     | 0.42              |
| 1:1A:5023:C:C3'    | 1:1A:5024:C:H4'    | 2.33                     | 0.42              |
| 3:1C:66:A:H2'      | 3:1C:67:U:H6       | 1.85                     | 0.42              |
| 5:1E:393:LYS:HG2   | 5:1E:396:ARG:HH21  | 1.84                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:1G:120:GLU:O    | 7:1G:248:ARG:NH1   | 2.47                     | 0.42              |
| 7:1G:129:GLU:HB2  | 7:1G:177:THR:CG2   | 2.49                     | 0.42              |
| 7:1G:234:ASP:C    | 7:1G:235:MET:HG3   | 2.41                     | 0.42              |
| 8:1H:93:THR:HG23  | 8:1H:104:THR:HB    | 2.00                     | 0.42              |
| 8:1H:136:HIS:HB2  | 8:1H:138:ARG:HH21  | 1.83                     | 0.42              |
| 11:2C:60:TRP:CE3  | 11:2C:60:TRP:HA    | 2.55                     | 0.42              |
| 14:2F:139:SER:O   | 14:2F:143:GLU:HG3  | 2.20                     | 0.42              |
| 20:2L:103:ARG:HG2 | 20:2L:124:TYR:CE2  | 2.54                     | 0.42              |
| 22:2N:111:GLU:C   | 22:2N:111:GLU:CD   | 2.87                     | 0.42              |
| 23:2O:95:ASN:HD22 | 23:2O:95:ASN:C     | 2.14                     | 0.42              |
| 30:2V:91:ARG:N    | 30:2V:91:ARG:HD2   | 2.35                     | 0.42              |
| 37:2c:79:THR:HG22 | 37:2c:81:ILE:HG22  | 2.01                     | 0.42              |
| 40:2f:33:ASN:HD21 | 40:2f:35:ILE:HG23  | 1.84                     | 0.42              |
| 46:2l:136:SER:O   | 46:2l:139:THR:HG22 | 2.20                     | 0.42              |
| 47:2m:113:G:OP1   | 47:2m:113:G:H2'    | 2.19                     | 0.42              |
| 47:2m:319:C:H5''  | 47:2m:320:G:OP2    | 2.19                     | 0.42              |
| 47:2m:415:A:H2'   | 47:2m:416:U:C6     | 2.54                     | 0.42              |
| 47:2m:959:G:H2'   | 47:2m:960:U:C6     | 2.54                     | 0.42              |
| 47:2m:963:A:O2'   | 47:2m:964:A:H5'    | 2.20                     | 0.42              |
| 47:2m:1089:G:H2'  | 47:2m:1090:C:H6    | 1.82                     | 0.42              |
| 47:2m:1262:C:C5   | 67:3E:17:GLY:HA3   | 2.53                     | 0.42              |
| 47:2m:1388:A:C2   | 47:2m:1389:C:H1'   | 2.55                     | 0.42              |
| 47:2m:1521:C:OP2  | 47:2m:1521:C:H6    | 2.03                     | 0.42              |
| 47:2m:1648:G:H8   | 58:2x:125:ARG:HB2  | 1.85                     | 0.42              |
| 48:2n:23:THR:HG1  | 48:2n:174:MET:HE1  | 1.85                     | 0.42              |
| 50:2p:22:ASN:O    | 50:2p:26:THR:OG1   | 2.33                     | 0.42              |
| 52:2r:19:LEU:HD23 | 52:2r:23:TRP:HB2   | 2.00                     | 0.42              |
| 55:2u:74:GLU:CD   | 55:2u:74:GLU:H     | 2.28                     | 0.42              |
| 63:3A:40:ASP:OD1  | 63:3A:43:THR:HG23  | 2.19                     | 0.42              |
| 63:3A:42:VAL:HG23 | 63:3A:43:THR:N     | 2.34                     | 0.42              |
| 66:3D:30:VAL:CB   | 66:3D:32:VAL:HG13  | 2.49                     | 0.42              |
| 69:3G:151:ILE:O   | 69:3G:155:ILE:HG13 | 2.19                     | 0.42              |
| 73:3K:63:VAL:CA   | 73:3K:66:VAL:HG12  | 2.45                     | 0.42              |
| 73:3K:150:VAL:O   | 73:3K:151:ALA:HB3  | 2.19                     | 0.42              |
| 1:1A:124:C:H2'    | 1:1A:125:C:C6      | 2.55                     | 0.42              |
| 1:1A:262:G:H2'    | 1:1A:263:G:C8      | 2.54                     | 0.42              |
| 1:1A:434:A:H3'    | 1:1A:435:A:H8      | 1.83                     | 0.42              |
| 1:1A:470:A:H61    | 1:1A:684:G:H1'     | 1.84                     | 0.42              |
| 1:1A:750:U:H1'    | 1:1A:917:A:C5      | 2.55                     | 0.42              |
| 1:1A:1308:C:O2    | 34:2Z:94:ALA:HB3   | 2.19                     | 0.42              |
| 1:1A:1308:C:OP1   | 17:2I:93:LYS:HD2   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1485:C:H4'   | 1:1A:1486:C:OP2   | 2.20                     | 0.42              |
| 1:1A:1575:A:O2'   | 1:1A:1576:G:H5'   | 2.20                     | 0.42              |
| 1:1A:1702:C:O2    | 1:1A:1702:C:O4'   | 2.35                     | 0.42              |
| 1:1A:1825:A:H2'   | 1:1A:1826:G:H8    | 1.85                     | 0.42              |
| 1:1A:1845:U:H2'   | 1:1A:1846:G:H8    | 1.84                     | 0.42              |
| 1:1A:1882:U:C4    | 1:1A:2279:A:C2    | 3.08                     | 0.42              |
| 1:1A:2606:G:H2'   | 1:1A:2607:C:C6    | 2.54                     | 0.42              |
| 1:1A:2608:G:O2'   | 1:1A:2609:G:H5'   | 2.18                     | 0.42              |
| 1:1A:2669:C:O2'   | 1:1A:2670:C:C5'   | 2.67                     | 0.42              |
| 1:1A:3834:C:H2'   | 1:1A:3835:C:H6    | 1.84                     | 0.42              |
| 1:1A:4071:U:O2'   | 1:1A:4072:C:H5'   | 2.20                     | 0.42              |
| 1:1A:4420:U:O4    | 1:1A:4475:G:N2    | 2.52                     | 0.42              |
| 1:1A:4869:U:HO2'  | 1:1A:4870:G:H5'   | 1.83                     | 0.42              |
| 1:1A:4873:G:H1    | 15:2G:98:ARG:HH21 | 1.65                     | 0.42              |
| 2:1B:31:G:C6      | 2:1B:47:G:C6      | 3.08                     | 0.42              |
| 2:1B:72:U:O2'     | 2:1B:73:U:H5'     | 2.19                     | 0.42              |
| 4:1D:142:GLU:C    | 4:1D:143:THR:HG23 | 2.44                     | 0.42              |
| 4:1D:178:PRO:CG   | 44:2j:26:VAL:HG23 | 2.48                     | 0.42              |
| 5:1E:139:ASP:O    | 5:1E:143:LYS:HE2  | 2.20                     | 0.42              |
| 7:1G:232:THR:OG1  | 7:1G:233:PRO:HD2  | 2.19                     | 0.42              |
| 12:2D:123:GLN:HG3 | 12:2D:124:GLY:N   | 2.34                     | 0.42              |
| 22:2N:97:LYS:HB3  | 22:2N:97:LYS:HE3  | 1.55                     | 0.42              |
| 28:2T:29:ILE:O    | 28:2T:30:ASP:HB2  | 2.19                     | 0.42              |
| 47:2m:813:A:C5    | 47:2m:814:U:C6    | 3.08                     | 0.42              |
| 47:2m:972:A:H3'   | 47:2m:973:C:C6    | 2.53                     | 0.42              |
| 47:2m:1263:U:C5'  | 67:3E:27:ARG:HH21 | 2.33                     | 0.42              |
| 47:2m:1309:C:H2'  | 47:2m:1310:U:C5   | 2.54                     | 0.42              |
| 47:2m:1396:A:H4'  | 47:2m:1396:A:OP1  | 2.19                     | 0.42              |
| 48:2n:41:ARG:HD2  | 48:2n:47:TYR:CE1  | 2.55                     | 0.42              |
| 49:2o:127:VAL:HB  | 49:2o:176:VAL:CG1 | 2.48                     | 0.42              |
| 50:2p:45:ARG:NH1  | 50:2p:82:GLY:O    | 2.51                     | 0.42              |
| 52:2r:171:GLU:H   | 52:2r:171:GLU:CD  | 2.27                     | 0.42              |
| 56:2v:82:MET:HG2  | 56:2v:82:MET:O    | 2.20                     | 0.42              |
| 59:2y:59:LYS:O    | 59:2y:62:GLN:NE2  | 2.49                     | 0.42              |
| 60:2z:67:VAL:C    | 60:2z:70:ILE:HG13 | 2.43                     | 0.42              |
| 60:2z:73:ASN:O    | 60:2z:73:ASN:CG   | 2.63                     | 0.42              |
| 61:20:22:LEU:HB3  | 61:20:28:LEU:CD2  | 2.50                     | 0.42              |
| 61:20:43:LYS:HG3  | 61:20:43:LYS:O    | 2.18                     | 0.42              |
| 68:3F:8:ARG:O     | 68:3F:8:ARG:CG    | 2.68                     | 0.42              |
| 69:3G:253:PRO:HG2 | 75:3M:99:PHE:HB3  | 2.00                     | 0.42              |
| 70:3H:152:ASP:OD2 | 70:3H:155:GLN:HB2 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 71:3I:132:GLN:O   | 71:3I:133:ARG:HB2  | 2.20                     | 0.42              |
| 76:3N:25:ILE:HD13 | 76:3N:60:PHE:HZ    | 1.85                     | 0.42              |
| 77:3O:70:PRO:HA   | 77:3O:73:VAL:HG12  | 2.01                     | 0.42              |
| 1:1A:128:C:H2'    | 1:1A:129:C:C1'     | 2.50                     | 0.42              |
| 1:1A:301:G:H2'    | 1:1A:302:C:C6      | 2.55                     | 0.42              |
| 1:1A:418:A:O5'    | 1:1A:418:A:H8      | 2.03                     | 0.42              |
| 1:1A:453:G:N3     | 1:1A:453:G:C2'     | 2.80                     | 0.42              |
| 1:1A:700:G:C2     | 1:1A:701:G:C5      | 3.08                     | 0.42              |
| 1:1A:1415:G:H2'   | 1:1A:1416:G:H5'    | 2.02                     | 0.42              |
| 1:1A:1883:G:N3    | 1:1A:1883:G:H2'    | 2.35                     | 0.42              |
| 1:1A:2483:G:C3'   | 1:1A:2484:A:H5''   | 2.50                     | 0.42              |
| 1:1A:2837:U:H2'   | 1:1A:2838:G:O4'    | 2.20                     | 0.42              |
| 1:1A:3598:C:H2'   | 1:1A:3599:A:C8     | 2.53                     | 0.42              |
| 1:1A:3615:G:H1'   | 25:2Q:44:ARG:HH21  | 1.85                     | 0.42              |
| 1:1A:3856:A:H2'   | 1:1A:3857:G:C8     | 2.55                     | 0.42              |
| 1:1A:3955:G:H2'   | 1:1A:3955:G:N3     | 2.35                     | 0.42              |
| 1:1A:4095:G:H2'   | 1:1A:4096:C:C5     | 2.55                     | 0.42              |
| 1:1A:4101:C:C2'   | 1:1A:4102:C:H5     | 2.31                     | 0.42              |
| 1:1A:4121:G:H21   | 4:1D:46:LYS:NZ     | 2.18                     | 0.42              |
| 1:1A:4572:U:H2'   | 1:1A:4573:G:C8     | 2.55                     | 0.42              |
| 1:1A:4678:G:H21   | 1:1A:4713:G:H1'    | 1.81                     | 0.42              |
| 1:1A:4749:C:O2    | 1:1A:4749:C:O4'    | 2.38                     | 0.42              |
| 1:1A:5030:U:H2'   | 1:1A:5031:G:H8     | 1.85                     | 0.42              |
| 2:1B:66:G:OP1     | 7:1G:10:LYS:HD2    | 2.20                     | 0.42              |
| 3:1C:69:U:H2'     | 3:1C:70:G:C8       | 2.55                     | 0.42              |
| 5:1E:297:LYS:HA   | 5:1E:297:LYS:HE3   | 2.01                     | 0.42              |
| 5:1E:321:VAL:O    | 5:1E:322:HIS:HB2   | 2.20                     | 0.42              |
| 6:1F:3:CYS:O      | 6:1F:3:CYS:SG      | 2.77                     | 0.42              |
| 6:1F:150:LEU:HB3  | 6:1F:151:PRO:HD3   | 2.00                     | 0.42              |
| 9:2A:92:VAL:HG13  | 9:2A:142:TRP:HB3   | 2.01                     | 0.42              |
| 9:2A:94:ARG:CZ    | 9:2A:109:LEU:HD13  | 2.50                     | 0.42              |
| 9:2A:175:ILE:HD11 | 9:2A:187:MET:SD    | 2.60                     | 0.42              |
| 10:2B:191:GLY:HA2 | 10:2B:194:VAL:HG22 | 2.02                     | 0.42              |
| 11:2C:140:GLN:NE2 | 11:2C:143:GLU:OE2  | 2.41                     | 0.42              |
| 13:2E:96:LYS:HG3  | 13:2E:174:ILE:HG21 | 2.02                     | 0.42              |
| 20:2L:4:LEU:HD21  | 20:2L:33:ALA:HB2   | 2.02                     | 0.42              |
| 23:2O:72:VAL:CB   | 23:2O:83:LEU:HD21  | 2.50                     | 0.42              |
| 26:2R:37:LYS:O    | 26:2R:37:LYS:HD2   | 2.20                     | 0.42              |
| 31:2W:78:ASN:OD1  | 31:2W:78:ASN:N     | 2.51                     | 0.42              |
| 34:2Z:105:LEU:O   | 34:2Z:105:LEU:CG   | 2.68                     | 0.42              |
| 47:2m:689:U:O4    | 53:2s:122:LEU:HD11 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:1644:C:H2'  | 47:2m:1645:C:H6    | 1.83                     | 0.42              |
| 47:2m:1644:C:OP1  | 58:2x:143:LYS:HB2  | 2.20                     | 0.42              |
| 48:2n:8:LEU:HD12  | 48:2n:8:LEU:O      | 2.19                     | 0.42              |
| 48:2n:88:LEU:HD12 | 48:2n:88:LEU:HA    | 1.87                     | 0.42              |
| 49:2o:110:MET:HA  | 49:2o:110:MET:HE3  | 2.01                     | 0.42              |
| 51:2q:122:LYS:HB3 | 51:2q:164:LEU:HD21 | 2.02                     | 0.42              |
| 51:2q:247:THR:O   | 51:2q:250:GLU:HG2  | 2.19                     | 0.42              |
| 52:2r:55:ARG:NH2  | 58:2x:125:ARG:HD3  | 2.35                     | 0.42              |
| 52:2r:78:MET:HG3  | 52:2r:78:MET:O     | 2.19                     | 0.42              |
| 52:2r:179:ASN:CG  | 52:2r:184:SER:HG   | 2.24                     | 0.42              |
| 54:2t:125:LYS:HB3 | 54:2t:128:LYS:HZ3  | 1.85                     | 0.42              |
| 58:2x:97:GLN:HE22 | 68:3F:58:ALA:HB3   | 1.85                     | 0.42              |
| 59:2y:93:GLN:C    | 59:2y:95:ILE:H     | 2.27                     | 0.42              |
| 60:2z:98:VAL:HG23 | 60:2z:103:LEU:HB2  | 2.01                     | 0.42              |
| 62:21:78:ASP:OD1  | 67:3E:54:LYS:HD3   | 2.20                     | 0.42              |
| 65:3C:41:ILE:O    | 65:3C:41:ILE:HG23  | 2.19                     | 0.42              |
| 70:3H:3:LEU:HB3   | 70:3H:5:ILE:CD1    | 2.44                     | 0.42              |
| 72:3J:93:LYS:HD2  | 72:3J:93:LYS:HA    | 1.92                     | 0.42              |
| 75:3M:19:LYS:HD3  | 75:3M:19:LYS:HA    | 1.93                     | 0.42              |
| 77:3O:63:PRO:HB2  | 77:3O:96:LEU:CD1   | 2.50                     | 0.42              |
| 79:3Q:28:LYS:HB3  | 79:3Q:32:ALA:HB1   | 1.99                     | 0.42              |
| 1:1A:25:A:C8      | 1:1A:341:G:C8      | 3.08                     | 0.42              |
| 1:1A:74:G:C5'     | 14:2F:59:VAL:HG13  | 2.43                     | 0.42              |
| 1:1A:667:A:C5     | 6:1F:291:ARG:NH2   | 2.88                     | 0.42              |
| 1:1A:685:C:H5''   | 1:1A:686:A:OP1     | 2.20                     | 0.42              |
| 1:1A:1297:U:O3'   | 34:2Z:58:VAL:HG13  | 2.19                     | 0.42              |
| 1:1A:1465:G:N2    | 1:1A:1466:G:H1'    | 2.34                     | 0.42              |
| 1:1A:1685:G:H2'   | 1:1A:1686:C:H6     | 1.85                     | 0.42              |
| 1:1A:1699:A:O3'   | 6:1F:306:ARG:NH1   | 2.53                     | 0.42              |
| 1:1A:1803:G:C6    | 22:2N:109:VAL:HG22 | 2.55                     | 0.42              |
| 1:1A:1882:U:H1'   | 1:1A:1883:G:C8     | 2.54                     | 0.42              |
| 1:1A:2690:C:O2'   | 1:1A:2691:U:H5'    | 2.20                     | 0.42              |
| 1:1A:3693:U:C4    | 1:1A:3694:U:C5     | 3.07                     | 0.42              |
| 1:1A:3909:C:O2    | 1:1A:4396:A:N1     | 2.53                     | 0.42              |
| 1:1A:4610:A:C4    | 1:1A:4611:A:C8     | 3.07                     | 0.42              |
| 1:1A:4757:C:O2    | 1:1A:4757:C:O4'    | 2.36                     | 0.42              |
| 1:1A:4970:C:H1'   | 1:1A:5064:G:N2     | 2.33                     | 0.42              |
| 3:1C:8:U:H2'      | 3:1C:9:A:H8        | 1.83                     | 0.42              |
| 9:2A:50:ILE:HG13  | 9:2A:51:TYR:N      | 2.35                     | 0.42              |
| 10:2B:80:ILE:HD11 | 16:2H:18:VAL:HG13  | 2.01                     | 0.42              |
| 14:2F:8:MET:SD    | 19:2K:168:ARG:HA   | 2.60                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:2H:178:HIS:HA   | 16:2H:181:HIS:CE1  | 2.55                     | 0.42              |
| 17:2I:197:LYS:HA   | 17:2I:201:LEU:O    | 2.19                     | 0.42              |
| 23:2O:106:SER:OG   | 23:2O:109:SER:HB3  | 2.20                     | 0.42              |
| 27:2S:45:ARG:HB2   | 27:2S:126:ARG:HH22 | 1.85                     | 0.42              |
| 35:2a:106:VAL:O    | 35:2a:110:GLN:HG3  | 2.20                     | 0.42              |
| 36:2b:46:LYS:O     | 36:2b:50:VAL:HG23  | 2.20                     | 0.42              |
| 40:2f:33:ASN:ND2   | 40:2f:35:ILE:HG23  | 2.35                     | 0.42              |
| 43:2i:74:GLU:OE2   | 43:2i:76:ASN:HB3   | 2.19                     | 0.42              |
| 46:2l:65:VAL:HG12  | 46:2l:111:LEU:CD1  | 2.49                     | 0.42              |
| 47:2m:849:A:H2'    | 47:2m:850:C:C6     | 2.55                     | 0.42              |
| 47:2m:1018:U:H2'   | 47:2m:1019:C:C6    | 2.55                     | 0.42              |
| 47:2m:1258:A:N1    | 47:2m:1663:A:H2'   | 2.34                     | 0.42              |
| 47:2m:1507:G:N1    | 80:3R:90:LYS:HA    | 2.20                     | 0.42              |
| 47:2m:1535:U:O2'   | 52:2r:88:MET:SD    | 2.74                     | 0.42              |
| 47:2m:1712:A:O2'   | 47:2m:1713:C:H5'   | 2.20                     | 0.42              |
| 47:2m:1859:A:P     | 65:3C:10:ARG:HH12  | 2.42                     | 0.42              |
| 49:2o:27:LYS:HA    | 49:2o:51:ARG:NH2   | 2.34                     | 0.42              |
| 50:2p:34:TYR:OH    | 50:2p:37:VAL:HG13  | 2.20                     | 0.42              |
| 50:2p:96:LEU:HG    | 50:2p:190:LEU:HD22 | 2.00                     | 0.42              |
| 50:2p:190:LEU:HD12 | 50:2p:200:PRO:HD3  | 2.01                     | 0.42              |
| 52:2r:128:ILE:HG23 | 66:3D:23:SER:HB3   | 2.02                     | 0.42              |
| 54:2t:141:ARG:HG2  | 54:2t:145:ILE:HD11 | 2.01                     | 0.42              |
| 55:2u:92:ALA:HB1   | 55:2u:96:ARG:HG3   | 2.01                     | 0.42              |
| 57:2w:45:LEU:CD2   | 57:2w:49:LEU:HD13  | 2.50                     | 0.42              |
| 59:2y:87:GLU:HG2   | 59:2y:88:VAL:N     | 2.35                     | 0.42              |
| 61:20:18:LEU:O     | 61:20:18:LEU:HD12  | 2.19                     | 0.42              |
| 61:20:85:ASN:CB    | 61:20:88:MET:HB2   | 2.50                     | 0.42              |
| 66:3D:10:LYS:HE3   | 66:3D:34:PHE:CE2   | 2.55                     | 0.42              |
| 66:3D:30:VAL:HG13  | 66:3D:46:VAL:HG12  | 2.01                     | 0.42              |
| 68:3F:176:VAL:HG12 | 68:3F:186:THR:CB   | 2.50                     | 0.42              |
| 69:3G:96:PHE:CD1   | 69:3G:96:PHE:C     | 2.97                     | 0.42              |
| 70:3H:32:MET:HB3   | 70:3H:65:GLN:HE22  | 1.83                     | 0.42              |
| 70:3H:64:LYS:CD    | 70:3H:82:SER:HB3   | 2.49                     | 0.42              |
| 73:3K:13:GLN:HE21  | 78:3P:21:LYS:HZ1   | 1.66                     | 0.42              |
| 75:3M:55:ASP:OD2   | 75:3M:57:ARG:HD3   | 2.20                     | 0.42              |
| 1:1A:93:G:H2'      | 1:1A:94:A:H8       | 1.77                     | 0.42              |
| 1:1A:122:U:O2      | 1:1A:122:U:H2'     | 2.19                     | 0.42              |
| 1:1A:277:G:O2'     | 1:1A:278:G:OP2     | 2.33                     | 0.42              |
| 1:1A:1176:C:O2'    | 1:1A:1177:U:H5'    | 2.19                     | 0.42              |
| 1:1A:1410:U:H3     | 30:2V:52:LYS:NZ    | 2.18                     | 0.42              |
| 1:1A:1794:A:H5''   | 1:1A:4214:A:H61    | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2262:G:N3     | 1:1A:2262:G:C2'    | 2.83                     | 0.42              |
| 1:1A:2268:A:H4'    | 1:1A:2270:G:C8     | 2.55                     | 0.42              |
| 1:1A:2408:U:O4'    | 1:1A:2409:U:C5     | 2.73                     | 0.42              |
| 1:1A:2410:C:H2'    | 1:1A:2410:C:O2     | 2.20                     | 0.42              |
| 1:1A:2447:U:O2'    | 1:1A:2448:G:H5'    | 2.20                     | 0.42              |
| 1:1A:4484:A:C2     | 1:1A:4485:C:C5     | 3.08                     | 0.42              |
| 2:1B:47:G:OP1      | 7:1G:94:ASN:HB2    | 2.19                     | 0.42              |
| 3:1C:151:G:OP2     | 10:2B:65:ARG:NE    | 2.35                     | 0.42              |
| 5:1E:397:ILE:HG13  | 5:1E:398:ALA:H     | 1.84                     | 0.42              |
| 11:2C:18:ILE:HG22  | 11:2C:27:VAL:HA    | 2.01                     | 0.42              |
| 15:2G:39:ASP:OD2   | 15:2G:70:GLN:HG3   | 2.20                     | 0.42              |
| 21:2M:81:TRP:O     | 21:2M:127:MET:HG2  | 2.20                     | 0.42              |
| 21:2M:97:TYR:CZ    | 21:2M:109:CYS:HA   | 2.54                     | 0.42              |
| 22:2N:19:PHE:CE2   | 22:2N:20:ARG:HG3   | 2.55                     | 0.42              |
| 25:2Q:66:GLU:O     | 25:2Q:66:GLU:HG2   | 2.20                     | 0.42              |
| 27:2S:44:VAL:CG1   | 27:2S:122:LYS:HD3  | 2.50                     | 0.42              |
| 31:2W:21:VAL:HG22  | 31:2W:101:ASP:OD1  | 2.20                     | 0.42              |
| 39:2e:68:GLU:N     | 39:2e:68:GLU:CD    | 2.77                     | 0.42              |
| 47:2m:29:G:H2'     | 47:2m:30:C:C6      | 2.54                     | 0.42              |
| 47:2m:85:A:H2'     | 47:2m:86:C:H6      | 1.85                     | 0.42              |
| 47:2m:94:G:OP1     | 51:2q:6:LYS:NZ     | 2.37                     | 0.42              |
| 47:2m:143:U:H5''   | 70:3H:180:VAL:HG22 | 2.02                     | 0.42              |
| 47:2m:642:U:O2'    | 47:2m:644:G:H4'    | 2.19                     | 0.42              |
| 47:2m:1613:G:H3'   | 57:2w:39:ALA:HB2   | 2.02                     | 0.42              |
| 47:2m:1738:C:OP1   | 70:3H:92:ARG:NH1   | 2.51                     | 0.42              |
| 47:2m:1739:C:H2'   | 47:2m:1740:C:C6    | 2.55                     | 0.42              |
| 47:2m:1834:A:N3    | 47:2m:1834:A:C2'   | 2.83                     | 0.42              |
| 48:2n:65:ILE:HG21  | 48:2n:182:VAL:CG2  | 2.50                     | 0.42              |
| 48:2n:140:VAL:O    | 48:2n:141:ASN:OD1  | 2.38                     | 0.42              |
| 49:2o:124:HIS:HA   | 49:2o:137:LEU:O    | 2.20                     | 0.42              |
| 51:2q:128:LYS:HG2  | 51:2q:130:PHE:CD1  | 2.54                     | 0.42              |
| 51:2q:136:ILE:HD11 | 51:2q:138:HIS:CE1  | 2.55                     | 0.42              |
| 51:2q:159:THR:HB   | 51:2q:173:ILE:HD11 | 2.02                     | 0.42              |
| 52:2r:73:THR:CG2   | 52:2r:86:LYS:HE3   | 2.50                     | 0.42              |
| 52:2r:126:THR:HA   | 52:2r:135:ARG:CZ   | 2.50                     | 0.42              |
| 53:2s:100:ILE:CD1  | 53:2s:122:LEU:HA   | 2.50                     | 0.42              |
| 56:2v:125:ILE:HB   | 56:2v:146:THR:OG1  | 2.19                     | 0.42              |
| 61:20:4:VAL:CG2    | 61:20:136:GLY:HA2  | 2.48                     | 0.42              |
| 64:3B:66:ILE:O     | 64:3B:68:LYS:NZ    | 2.39                     | 0.42              |
| 68:3F:88:ARG:HH21  | 68:3F:100:ARG:HE   | 1.68                     | 0.42              |
| 73:3K:83:ASP:OD2   | 73:3K:84:LEU:HD12  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 76:3N:63:HIS:CE1  | 76:3N:68:LYS:HE3   | 2.55                     | 0.42              |
| 76:3N:110:ARG:HD3 | 76:3N:126:GLY:O    | 2.20                     | 0.42              |
| 1:1A:693:C:H2'    | 1:1A:694:C:C6      | 2.55                     | 0.41              |
| 1:1A:1187:G:H2'   | 1:1A:1188:C:H6     | 1.85                     | 0.41              |
| 1:1A:1964:A:H2'   | 1:1A:1965:G:O4'    | 2.20                     | 0.41              |
| 1:1A:2038:U:H2'   | 1:1A:2039:G:O4'    | 2.20                     | 0.41              |
| 1:1A:2426:U:O2'   | 1:1A:2427:G:H5'    | 2.19                     | 0.41              |
| 1:1A:2640:G:H2'   | 1:1A:2641:A:C8     | 2.55                     | 0.41              |
| 1:1A:2732:G:H2'   | 1:1A:2733:C:H6     | 1.83                     | 0.41              |
| 1:1A:3597:G:N7    | 20:2L:114:LYS:NZ   | 2.67                     | 0.41              |
| 1:1A:3618:C:H6    | 1:1A:3618:C:H3'    | 1.85                     | 0.41              |
| 1:1A:3867:A:O2'   | 1:1A:3868:G:H5'    | 2.19                     | 0.41              |
| 1:1A:4228:G:H5''  | 1:1A:4229:U:O4'    | 2.19                     | 0.41              |
| 1:1A:4748:U:H3    | 1:1A:4951:G:H1     | 1.68                     | 0.41              |
| 1:1A:4863:G:C2    | 1:1A:4864:U:H1'    | 2.55                     | 0.41              |
| 1:1A:4951:G:C2    | 1:1A:4952:G:C8     | 3.08                     | 0.41              |
| 9:2A:220:MET:O    | 9:2A:221:LYS:HG2   | 2.21                     | 0.41              |
| 10:2B:180:PRO:HA  | 10:2B:227:ASN:OD1  | 2.20                     | 0.41              |
| 13:2E:130:PHE:N   | 13:2E:130:PHE:CD1  | 2.88                     | 0.41              |
| 20:2L:24:LEU:HD23 | 20:2L:50:ILE:HG12  | 2.01                     | 0.41              |
| 20:2L:28:GLU:HG3  | 20:2L:49:LEU:HG    | 2.01                     | 0.41              |
| 25:2Q:78:PHE:CD1  | 70:3H:9:ALA:HA     | 2.55                     | 0.41              |
| 39:2e:22:SER:HB2  | 39:2e:65:ALA:HB3   | 2.01                     | 0.41              |
| 46:2l:85:MET:CE   | 46:2l:86:ASP:O     | 2.68                     | 0.41              |
| 47:2m:287:U:O2    | 51:2q:131:VAL:HG21 | 2.20                     | 0.41              |
| 47:2m:337:C:H3'   | 47:2m:338:G:H5''   | 2.02                     | 0.41              |
| 47:2m:502:C:C5    | 51:2q:66:MET:HB3   | 2.55                     | 0.41              |
| 47:2m:609:U:H2'   | 47:2m:610:G:H8     | 1.84                     | 0.41              |
| 47:2m:655:A:C5'   | 47:2m:656:G:H5'    | 2.50                     | 0.41              |
| 47:2m:1144:A:C5'  | 47:2m:1355:C:H41   | 2.20                     | 0.41              |
| 47:2m:1232:U:H2'  | 47:2m:1233:G:H8    | 1.84                     | 0.41              |
| 47:2m:1269:G:H2'  | 47:2m:1270:G:O4'   | 2.19                     | 0.41              |
| 47:2m:1271:C:OP2  | 80:3R:92:LYS:HD3   | 2.20                     | 0.41              |
| 47:2m:1279:C:H2'  | 47:2m:1280:G:C1'   | 2.50                     | 0.41              |
| 47:2m:1287:A:H5'' | 47:2m:1288:U:C4    | 2.55                     | 0.41              |
| 47:2m:1404:U:O2   | 47:2m:1580:A:H3'   | 2.20                     | 0.41              |
| 47:2m:1576:G:H2'  | 47:2m:1577:G:H8    | 1.84                     | 0.41              |
| 51:2q:48:LEU:CD2  | 51:2q:52:LEU:HD12  | 2.50                     | 0.41              |
| 56:2v:104:LYS:HE2 | 64:3B:8:ARG:NH2    | 2.35                     | 0.41              |
| 58:2x:62:ARG:HG2  | 58:2x:62:ARG:HH11  | 1.84                     | 0.41              |
| 59:2y:71:ILE:H    | 59:2y:71:ILE:CD1   | 2.30                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:20:43:LYS:HZ3  | 61:20:47:PRO:HG3   | 1.85                     | 0.41              |
| 68:3F:8:ARG:HG2   | 68:3F:311:GLN:HE21 | 1.85                     | 0.41              |
| 69:3G:75:ILE:HD11 | 69:3G:265:PRO:HB3  | 2.01                     | 0.41              |
| 70:3H:143:LYS:HG2 | 70:3H:144:LEU:N    | 2.35                     | 0.41              |
| 72:3J:97:GLU:O    | 72:3J:97:GLU:HG2   | 2.20                     | 0.41              |
| 80:3R:131:PHE:CD1 | 80:3R:131:PHE:N    | 2.88                     | 0.41              |
| 1:1A:954:C:O2'    | 1:1A:955:G:H5'     | 2.20                     | 0.41              |
| 1:1A:990:C:N3     | 1:1A:992:C:H1'     | 2.35                     | 0.41              |
| 1:1A:1178:G:H2'   | 1:1A:1178:G:N3     | 2.35                     | 0.41              |
| 1:1A:1646:A:H2'   | 1:1A:1647:U:C6     | 2.55                     | 0.41              |
| 1:1A:1777:C:H2'   | 1:1A:1778:C:C6     | 2.55                     | 0.41              |
| 1:1A:1980:U:OP1   | 1:1A:1982:G:H5''   | 2.20                     | 0.41              |
| 1:1A:2020:U:H2'   | 1:1A:2021:G:C5'    | 2.49                     | 0.41              |
| 1:1A:2034:G:C4    | 1:1A:2035:C:C5     | 3.07                     | 0.41              |
| 1:1A:2098:G:O2'   | 1:1A:2099:G:O4'    | 2.39                     | 0.41              |
| 1:1A:2529:A:H4'   | 1:1A:2529:A:OP1    | 2.19                     | 0.41              |
| 1:1A:2614:C:O2'   | 1:1A:2808:G:OP1    | 2.38                     | 0.41              |
| 1:1A:2677:G:C2'   | 1:1A:2678:A:H5'    | 2.50                     | 0.41              |
| 1:1A:2682:G:H2'   | 1:1A:2683:C:H6     | 1.84                     | 0.41              |
| 1:1A:2847:G:C2'   | 1:1A:2848:G:H5'    | 2.50                     | 0.41              |
| 1:1A:4181:U:O2'   | 1:1A:4182:G:H5'    | 2.20                     | 0.41              |
| 1:1A:4501:U:OP2   | 1:1A:4502:C:H5     | 2.03                     | 0.41              |
| 1:1A:4674:C:H2'   | 1:1A:4675:U:C6     | 2.55                     | 0.41              |
| 1:1A:4899:G:N1    | 1:1A:4901:G:N7     | 2.67                     | 0.41              |
| 1:1A:4933:C:O2'   | 1:1A:4934:A:H5'    | 2.20                     | 0.41              |
| 5:1E:27:GLY:HA2   | 5:1E:276:HIS:CD2   | 2.55                     | 0.41              |
| 6:1F:174:LEU:O    | 6:1F:175:LYS:HB2   | 2.20                     | 0.41              |
| 7:1G:37:VAL:HG23  | 7:1G:50:ARG:HD3    | 2.01                     | 0.41              |
| 7:1G:117:LYS:CE   | 7:1G:117:LYS:HA    | 2.49                     | 0.41              |
| 7:1G:144:CYS:SG   | 7:1G:173:ILE:HG12  | 2.60                     | 0.41              |
| 8:1H:94:LYS:HB3   | 8:1H:94:LYS:HE2    | 1.86                     | 0.41              |
| 10:2B:159:HIS:NE2 | 10:2B:185:LYS:HD2  | 2.35                     | 0.41              |
| 11:2C:141:LYS:HG3 | 11:2C:142:ASP:CG   | 2.45                     | 0.41              |
| 12:2D:55:ASP:OD2  | 12:2D:162:ARG:HD3  | 2.20                     | 0.41              |
| 13:2E:99:PHE:HB2  | 13:2E:159:LYS:HE3  | 2.02                     | 0.41              |
| 20:2L:149:LYS:HE2 | 20:2L:149:LYS:HB2  | 1.84                     | 0.41              |
| 24:2P:43:LYS:HG3  | 24:2P:60:MET:HG2   | 2.01                     | 0.41              |
| 30:2V:65:MET:HG2  | 30:2V:68:ARG:HH21  | 1.85                     | 0.41              |
| 41:2g:104:HIS:HB2 | 41:2g:105:PRO:HD2  | 2.02                     | 0.41              |
| 46:2l:53:VAL:O    | 46:2l:154:THR:HG21 | 2.20                     | 0.41              |
| 46:2l:147:LYS:NZ  | 46:2l:150:GLU:H    | 2.18                     | 0.41              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 47:2m:165:G:C2'      | 47:2m:166:A:H5'    | 2.50                     | 0.41              |
| 47:2m:560:A:P        | 71:3I:174:LYS:HG3  | 2.60                     | 0.41              |
| 47:2m:1222:G:H5''    | 52:2r:78:MET:CE    | 2.50                     | 0.41              |
| 47:2m:1236:G:O2'     | 57:2w:131:PRO:HA   | 2.20                     | 0.41              |
| 47:2m:1270:G:OP2     | 47:2m:1270:G:H8    | 2.03                     | 0.41              |
| 47:2m:1457:U:H2'     | 47:2m:1458:G:H8    | 1.80                     | 0.41              |
| 47:2m:1461:G:H21     | 47:2m:1464:C:H3'   | 1.85                     | 0.41              |
| 47:2m:1717:C:C2'     | 47:2m:1718:G:H5'   | 2.50                     | 0.41              |
| 47:2m:1735:A:H2'     | 47:2m:1736:G:O4'   | 2.19                     | 0.41              |
| 48:2n:30:LEU:HB2     | 48:2n:47:TYR:CE2   | 2.55                     | 0.41              |
| 52:2r:35:LEU:O       | 52:2r:39:ILE:HB    | 2.20                     | 0.41              |
| 52:2r:56:TYR:CZ      | 52:2r:66:CYS:HA    | 2.55                     | 0.41              |
| 52:2r:61:PHE:CD2     | 66:3D:51:ARG:HG3   | 2.55                     | 0.41              |
| 52:2r:102:LEU:N      | 52:2r:102:LEU:HD23 | 2.33                     | 0.41              |
| 52:2r:142:SER:HA     | 66:3D:56:LEU:CD2   | 2.49                     | 0.41              |
| 53:2s:10:LYS:CD      | 53:2s:45:ILE:HD11  | 2.50                     | 0.41              |
| 54:2t:191:GLU:HA     | 54:2t:195:LEU:HB2  | 2.02                     | 0.41              |
| 57:2w:108:LYS:HD3    | 57:2w:109:PRO:CD   | 2.49                     | 0.41              |
| 58:2x:17:LYS:HG2     | 58:2x:125:ARG:O    | 2.20                     | 0.41              |
| 60:2z:106:LYS:HD3    | 60:2z:109:GLU:OE2  | 2.19                     | 0.41              |
| 61:20:64:LEU:HD12    | 61:20:121:ARG:O    | 2.20                     | 0.41              |
| 63:3A:11:LEU:O       | 63:3A:11:LEU:HD13  | 2.20                     | 0.41              |
| 65:3C:22:ARG:NH2     | 74:3L:145:GLY:O    | 2.53                     | 0.41              |
| 71:3I:138[A]:ARG:HB2 | 71:3I:139:LYS:HD3  | 2.02                     | 0.41              |
| 72:3J:18:LEU:CD1     | 72:3J:77:ILE:HD13  | 2.50                     | 0.41              |
| 72:3J:131:LYS:HE3    | 72:3J:132:LYS:HE3  | 2.02                     | 0.41              |
| 74:3L:100:THR:CG2    | 74:3L:104:ARG:HD3  | 2.42                     | 0.41              |
| 1:1A:212:A:H2'       | 1:1A:213:G:H8      | 1.85                     | 0.41              |
| 1:1A:714:G:H2'       | 1:1A:715:G:H8      | 1.85                     | 0.41              |
| 1:1A:993:G:C6        | 1:1A:1050:C:H2'    | 2.56                     | 0.41              |
| 1:1A:1812:C:O2'      | 1:1A:1813:U:H5'    | 2.21                     | 0.41              |
| 1:1A:1886:G:H2'      | 1:1A:1887:G:H5'    | 2.02                     | 0.41              |
| 1:1A:1895:G:H2'      | 1:1A:1896:A:O4'    | 2.20                     | 0.41              |
| 1:1A:1899:G:O2'      | 33:2Y:59:GLY:HA3   | 2.20                     | 0.41              |
| 1:1A:1962:A:H5'      | 1:1A:1963:C:OP2    | 2.20                     | 0.41              |
| 1:1A:2749:C:H2'      | 1:1A:2750:G:C8     | 2.54                     | 0.41              |
| 1:1A:2862:G:H4'      | 1:1A:3625:G:N7     | 2.35                     | 0.41              |
| 1:1A:3604:A:H2'      | 1:1A:3605:C:H5'    | 2.02                     | 0.41              |
| 1:1A:3658:C:H4'      | 4:1D:240:ALA:CB    | 2.50                     | 0.41              |
| 1:1A:3680:U:OP1      | 4:1D:54:ARG:NH2    | 2.34                     | 0.41              |
| 1:1A:4305:G:N3       | 1:1A:4305:G:C2'    | 2.83                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:4564:A:H2'   | 1:1A:4565:C:C6     | 2.55                     | 0.41              |
| 1:1A:4712:C:O2'   | 1:1A:4713:G:H5'    | 2.20                     | 0.41              |
| 5:1E:390:GLY:O    | 5:1E:392:LEU:HD22  | 2.21                     | 0.41              |
| 15:2G:100:ARG:HG3 | 17:2I:200:GLY:CA   | 2.50                     | 0.41              |
| 15:2G:126:GLU:CG  | 17:2I:185:VAL:CG1  | 2.98                     | 0.41              |
| 16:2H:151:ILE:O   | 16:2H:151:ILE:HG13 | 2.20                     | 0.41              |
| 18:2J:84:PRO:HB2  | 18:2J:87:SER:HB2   | 2.02                     | 0.41              |
| 29:2U:14:HIS:ND1  | 29:2U:14:HIS:N     | 2.68                     | 0.41              |
| 32:2X:23:ARG:HB2  | 32:2X:25:TYR:CE1   | 2.55                     | 0.41              |
| 43:2i:57:ARG:HE   | 43:2i:57:ARG:HB3   | 1.62                     | 0.41              |
| 46:2l:107:TYR:O   | 46:2l:133:LYS:HD3  | 2.19                     | 0.41              |
| 47:2m:15:U:C2'    | 47:2m:16:G:H5'     | 2.50                     | 0.41              |
| 47:2m:165:G:H2'   | 47:2m:166:A:H5'    | 2.02                     | 0.41              |
| 47:2m:327:G:C4    | 47:2m:328:U:H1'    | 2.55                     | 0.41              |
| 47:2m:355:G:OP2   | 56:2v:107:LYS:NZ   | 2.48                     | 0.41              |
| 47:2m:550:C:H2'   | 47:2m:551:U:C5     | 2.55                     | 0.41              |
| 47:2m:571:U:O2    | 47:2m:571:U:H2'    | 2.20                     | 0.41              |
| 47:2m:604:A:H3'   | 47:2m:604:A:OP2    | 2.20                     | 0.41              |
| 47:2m:633:C:H4'   | 64:3B:88:ASP:OD2   | 2.20                     | 0.41              |
| 47:2m:752:G:H5'   | 47:2m:792:C:O2'    | 2.20                     | 0.41              |
| 47:2m:827:A:H2'   | 47:2m:827:A:N3     | 2.35                     | 0.41              |
| 47:2m:876:C:H5''  | 47:2m:877:C:OP1    | 2.20                     | 0.41              |
| 47:2m:919:A:P     | 73:3K:64:ARG:HH22  | 2.43                     | 0.41              |
| 47:2m:963:A:OP1   | 74:3L:65:ASP:HB3   | 2.20                     | 0.41              |
| 47:2m:1017:U:H2'  | 47:2m:1018:U:H6    | 1.85                     | 0.41              |
| 47:2m:1228:A:O2'  | 47:2m:1229:G:H5'   | 2.20                     | 0.41              |
| 47:2m:1391:C:C4'  | 67:3E:55:LEU:HD23  | 2.45                     | 0.41              |
| 47:2m:1422:G:H1'  | 47:2m:1424:G:H8    | 1.84                     | 0.41              |
| 47:2m:1650:A:C4   | 47:2m:1675:A:N6    | 2.89                     | 0.41              |
| 48:2n:3:GLY:N     | 48:2n:59:LEU:HD13  | 2.34                     | 0.41              |
| 50:2p:69:LEU:O    | 50:2p:73:VAL:HG23  | 2.21                     | 0.41              |
| 51:2q:36:HIS:HE1  | 51:2q:88:ASP:OD2   | 2.03                     | 0.41              |
| 51:2q:211:LYS:HB2 | 51:2q:211:LYS:HE3  | 1.55                     | 0.41              |
| 53:2s:7:LYS:HE2   | 53:2s:10:LYS:NZ    | 2.35                     | 0.41              |
| 57:2w:57:LEU:HB3  | 57:2w:61:ARG:NH2   | 2.36                     | 0.41              |
| 57:2w:108:LYS:CG  | 57:2w:109:PRO:HD2  | 2.50                     | 0.41              |
| 57:2w:111:MET:CB  | 60:2z:117:ILE:HG12 | 2.48                     | 0.41              |
| 59:2y:33:ARG:O    | 59:2y:37:GLU:HG3   | 2.21                     | 0.41              |
| 60:2z:47:LYS:HE2  | 60:2z:77:TYR:CG    | 2.55                     | 0.41              |
| 62:21:41:ARG:HA   | 62:21:44:LYS:HG2   | 2.02                     | 0.41              |
| 62:21:60:THR:OG1  | 62:21:83:ARG:HG2   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:21:106:ILE:HG23 | 62:21:107:GLU:N    | 2.35                     | 0.41              |
| 63:3A:19:ALA:HB2   | 63:3A:68:SER:HB2   | 2.02                     | 0.41              |
| 64:3B:37:LYS:CE    | 64:3B:37:LYS:HA    | 2.50                     | 0.41              |
| 64:3B:61:GLN:CB    | 64:3B:62:PRO:HD3   | 2.46                     | 0.41              |
| 66:3D:37:ASP:CB    | 66:3D:40:ARG:HG2   | 2.49                     | 0.41              |
| 69:3G:167:ARG:HG2  | 69:3G:219:ILE:HD13 | 2.02                     | 0.41              |
| 72:3J:68:LEU:HA    | 80:3R:114:ILE:CD1  | 2.42                     | 0.41              |
| 73:3K:91:LEU:HB3   | 73:3K:122:ILE:HG12 | 2.01                     | 0.41              |
| 74:3L:33:ILE:HA    | 74:3L:41:PHE:O     | 2.20                     | 0.41              |
| 76:3N:16:ARG:O     | 76:3N:19:GLN:HG3   | 2.20                     | 0.41              |
| 1:1A:123:C:H2'     | 1:1A:124:C:C6      | 2.53                     | 0.41              |
| 1:1A:254:G:O5'     | 1:1A:254:G:H8      | 2.04                     | 0.41              |
| 1:1A:717:U:O2'     | 1:1A:718:C:H5'     | 2.19                     | 0.41              |
| 1:1A:753:C:H5      | 1:1A:910:G:H1      | 1.68                     | 0.41              |
| 1:1A:972:C:O2      | 1:1A:972:C:H2'     | 2.21                     | 0.41              |
| 1:1A:1078:A:H2'    | 1:1A:1079:C:C5'    | 2.40                     | 0.41              |
| 1:1A:1254:A:N3     | 1:1A:1254:A:H2'    | 2.36                     | 0.41              |
| 1:1A:1294:A:H1'    | 1:1A:1296:G:H1     | 1.83                     | 0.41              |
| 1:1A:1598:C:H1'    | 1:1A:2798:A:C8     | 2.54                     | 0.41              |
| 1:1A:1706:A:N6     | 30:2V:101:HIS:HA   | 2.36                     | 0.41              |
| 1:1A:1754:U:O5'    | 1:1A:1754:U:H6     | 2.04                     | 0.41              |
| 1:1A:1936:C:C5     | 2:1B:84:U:C4       | 3.08                     | 0.41              |
| 1:1A:2718:U:C5'    | 1:1A:2719:C:H5'    | 2.51                     | 0.41              |
| 1:1A:2743:A:H2'    | 1:1A:2744:A:H8     | 1.84                     | 0.41              |
| 1:1A:3636:C:O2     | 1:1A:3636:C:H2'    | 2.21                     | 0.41              |
| 1:1A:3694:U:C4     | 1:1A:3695:U:C4     | 3.09                     | 0.41              |
| 1:1A:3906:A:O4'    | 1:1A:4448:G:H1'    | 2.20                     | 0.41              |
| 1:1A:3932:U:H2'    | 1:1A:3933:G:H8     | 1.85                     | 0.41              |
| 1:1A:4046:A:H3'    | 1:1A:4046:A:P      | 2.59                     | 0.41              |
| 1:1A:4096:C:H2'    | 1:1A:4097:G:H8     | 1.83                     | 0.41              |
| 1:1A:4168:G:C2'    | 1:1A:4169:G:H5'    | 2.50                     | 0.41              |
| 1:1A:4543:G:H2'    | 1:1A:4544:A:C8     | 2.54                     | 0.41              |
| 1:1A:4622:A:H4'    | 5:1E:13:SER:HB2    | 2.02                     | 0.41              |
| 1:1A:4982:A:OP1    | 18:2J:74:LYS:NZ    | 2.49                     | 0.41              |
| 1:1A:5005:G:N2     | 1:1A:5041:G:O2'    | 2.54                     | 0.41              |
| 2:1B:48:G:H5'      | 7:1G:226:TYR:HE1   | 1.86                     | 0.41              |
| 2:1B:74:A:O2'      | 21:2M:53:LYS:NZ    | 2.49                     | 0.41              |
| 3:1C:87:G:OP2      | 3:1C:87:G:H3'      | 2.20                     | 0.41              |
| 5:1E:107:ALA:CB    | 5:1E:201:LEU:HG    | 2.40                     | 0.41              |
| 5:1E:232:THR:O     | 5:1E:236:HIS:HA    | 2.20                     | 0.41              |
| 7:1G:228:LYS:HE2   | 7:1G:228:LYS:HB3   | 1.52                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:144:ILE:HG12  | 8:1H:196:ALA:HB2   | 2.02                     | 0.41              |
| 10:2B:244:PRO:HA   | 10:2B:247:VAL:HG22 | 2.01                     | 0.41              |
| 11:2C:144:LEU:HD12 | 11:2C:161:ILE:CD1  | 2.50                     | 0.41              |
| 15:2G:104:MET:HE3  | 15:2G:109:ARG:HA   | 2.01                     | 0.41              |
| 16:2H:48:ALA:C     | 16:2H:53:TYR:HB3   | 2.46                     | 0.41              |
| 24:2P:26:ILE:HB    | 24:2P:101:ASN:O    | 2.20                     | 0.41              |
| 27:2S:26:ARG:HG2   | 27:2S:78:TYR:CZ    | 2.56                     | 0.41              |
| 28:2T:89:ILE:HD11  | 28:2T:91:LEU:HD13  | 1.97                     | 0.41              |
| 29:2U:122:VAL:O    | 29:2U:142:GLY:HA3  | 2.20                     | 0.41              |
| 30:2V:75:LEU:O     | 30:2V:76:VAL:HB    | 2.20                     | 0.41              |
| 46:2l:65:VAL:CG1   | 46:2l:111:LEU:HA   | 2.50                     | 0.41              |
| 46:2l:86:ASP:OD1   | 46:2l:87:ILE:HG23  | 2.21                     | 0.41              |
| 47:2m:126:G:H1'    | 47:2m:127:C:H5''   | 2.02                     | 0.41              |
| 47:2m:141:A:H5''   | 47:2m:143:U:OP1    | 2.21                     | 0.41              |
| 47:2m:681:U:H4'    | 64:3B:9:THR:HG22   | 2.03                     | 0.41              |
| 47:2m:686:U:H2'    | 47:2m:687:C:O2     | 2.20                     | 0.41              |
| 47:2m:800:U:H2'    | 47:2m:801:U:O4'    | 2.20                     | 0.41              |
| 47:2m:809:A:H1'    | 47:2m:810:A:C2     | 2.56                     | 0.41              |
| 47:2m:834:C:H42    | 47:2m:839:C:N4     | 2.17                     | 0.41              |
| 47:2m:988:C:H5''   | 49:2o:116:LYS:HG2  | 2.03                     | 0.41              |
| 47:2m:1262:C:H5    | 67:3E:17:GLY:CA    | 2.33                     | 0.41              |
| 47:2m:1263:U:H4'   | 67:3E:27:ARG:NE    | 2.23                     | 0.41              |
| 47:2m:1368:U:H1'   | 59:2y:4:VAL:HG21   | 2.02                     | 0.41              |
| 47:2m:1705:C:H2'   | 47:2m:1706:G:H8    | 1.80                     | 0.41              |
| 48:2n:62:ALA:O     | 48:2n:65:ILE:HG22  | 2.20                     | 0.41              |
| 48:2n:85:ARG:HH21  | 48:2n:201:LEU:HA   | 1.85                     | 0.41              |
| 49:2o:69:VAL:CG1   | 49:2o:86:LEU:HD22  | 2.50                     | 0.41              |
| 51:2q:44:LEU:HD11  | 51:2q:90:ILE:HD13  | 2.01                     | 0.41              |
| 51:2q:159:THR:HB   | 51:2q:173:ILE:CD1  | 2.49                     | 0.41              |
| 52:2r:35:LEU:HD12  | 52:2r:143:PRO:CB   | 2.50                     | 0.41              |
| 54:2t:113:TYR:HD2  | 54:2t:121:LEU:HB3  | 1.85                     | 0.41              |
| 58:2x:86:GLN:HG2   | 58:2x:86:GLN:H     | 1.72                     | 0.41              |
| 65:3C:102:ARG:N    | 65:3C:103:PRO:HD2  | 2.35                     | 0.41              |
| 69:3G:199:PRO:O    | 69:3G:221:ASP:OD2  | 2.38                     | 0.41              |
| 69:3G:219:ILE:CG2  | 69:3G:222:CYS:HB2  | 2.51                     | 0.41              |
| 70:3H:140:ARG:CB   | 70:3H:143:LYS:HE2  | 2.51                     | 0.41              |
| 72:3J:14:VAL:HG13  | 72:3J:15:ASN:N     | 2.36                     | 0.41              |
| 74:3L:65:ASP:OD1   | 74:3L:65:ASP:C     | 2.63                     | 0.41              |
| 75:3M:42:MET:HG3   | 75:3M:48:GLY:O     | 2.21                     | 0.41              |
| 76:3N:5:VAL:O      | 76:3N:5:VAL:HG12   | 2.19                     | 0.41              |
| 78:3P:17:ARG:HG3   | 78:3P:17:ARG:NH1   | 2.35                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:65:A:H61     | 1:1A:75:G:H1'      | 1.86                     | 0.41              |
| 1:1A:88:A:N7      | 19:2K:173:LYS:NZ   | 2.69                     | 0.41              |
| 1:1A:191:G:O2'    | 1:1A:192:G:H5'     | 2.21                     | 0.41              |
| 1:1A:1318:C:C2'   | 1:1A:1319:U:H5'    | 2.50                     | 0.41              |
| 1:1A:1344:C:H1'   | 14:2F:10:LEU:HD11  | 2.01                     | 0.41              |
| 1:1A:1563:A:C6    | 47:2m:677:G:O2'    | 2.72                     | 0.41              |
| 1:1A:1669:A:H1'   | 1:1A:1852:U:O2'    | 2.21                     | 0.41              |
| 1:1A:1702:C:C4    | 1:1A:1703:C:C2     | 3.09                     | 0.41              |
| 1:1A:1970:A:H5'   | 1:1A:1971:C:O4'    | 2.19                     | 0.41              |
| 1:1A:2483:G:H5'   | 1:1A:2484:A:OP2    | 2.21                     | 0.41              |
| 1:1A:2728:U:O2'   | 1:1A:2729:C:H5'    | 2.20                     | 0.41              |
| 1:1A:2792:C:O2    | 38:2d:9:GLY:HA2    | 2.21                     | 0.41              |
| 1:1A:3896:C:O2'   | 5:1E:268:ARG:NH1   | 2.51                     | 0.41              |
| 1:1A:4122:G:C8    | 35:2a:97:ILE:HD12  | 2.54                     | 0.41              |
| 1:1A:4652:G:H2'   | 1:1A:4653:C:H6     | 1.84                     | 0.41              |
| 1:1A:4758:U:C2'   | 1:1A:4759:C:H5'    | 2.51                     | 0.41              |
| 1:1A:4761:G:O2'   | 1:1A:4762:A:H5'    | 2.20                     | 0.41              |
| 1:1A:4775:C:H2'   | 1:1A:4861:G:N2     | 2.36                     | 0.41              |
| 3:1C:17:A:C4      | 3:1C:18:U:C6       | 3.09                     | 0.41              |
| 3:1C:81:C:H5''    | 3:1C:82:A:OP1      | 2.20                     | 0.41              |
| 4:1D:33:ASP:OD1   | 4:1D:36:GLU:HB2    | 2.20                     | 0.41              |
| 5:1E:292:LEU:HD12 | 5:1E:292:LEU:HA    | 1.78                     | 0.41              |
| 8:1H:148:THR:HG22 | 8:1H:164:PHE:HB3   | 2.03                     | 0.41              |
| 9:2A:92:VAL:HG13  | 9:2A:140:ILE:HD12  | 2.02                     | 0.41              |
| 10:2B:60:TYR:CZ   | 10:2B:61:ILE:HG13  | 2.55                     | 0.41              |
| 10:2B:99:ALA:HB2  | 10:2B:204:PHE:HZ   | 1.86                     | 0.41              |
| 11:2C:27:VAL:HG23 | 11:2C:80:MET:HE2   | 2.02                     | 0.41              |
| 12:2D:89:VAL:HG12 | 12:2D:136:MET:HG3  | 2.00                     | 0.41              |
| 13:2E:158:SER:H   | 13:2E:161:GLU:CG   | 2.33                     | 0.41              |
| 15:2G:79:LYS:NZ   | 15:2G:79:LYS:HB2   | 2.35                     | 0.41              |
| 17:2I:145:VAL:O   | 17:2I:145:VAL:HG13 | 2.20                     | 0.41              |
| 35:2a:60:ARG:HA   | 35:2a:60:ARG:HD2   | 1.91                     | 0.41              |
| 35:2a:110:GLN:OE1 | 35:2a:111:ALA:N    | 2.54                     | 0.41              |
| 44:2j:90:LYS:HD3  | 44:2j:91:ASP:OD1   | 2.20                     | 0.41              |
| 46:2l:32:VAL:CG2  | 46:2l:206:ILE:HD11 | 2.50                     | 0.41              |
| 46:2l:74:CYS:O    | 46:2l:78:LYS:HE3   | 2.20                     | 0.41              |
| 47:2m:56:G:H2'    | 47:2m:57:U:C6      | 2.56                     | 0.41              |
| 47:2m:327:G:H1'   | 47:2m:328:U:H1'    | 2.03                     | 0.41              |
| 47:2m:352:U:C2    | 47:2m:353:C:C5     | 3.09                     | 0.41              |
| 47:2m:483:C:H5''  | 64:3B:48:LYS:CD    | 2.51                     | 0.41              |
| 47:2m:522:A:H5''  | 71:3I:145:PRO:HD2  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:621:C:H2'    | 47:2m:622:C:C6     | 2.54                     | 0.41              |
| 47:2m:841:G:C4     | 47:2m:842:C:C5     | 3.09                     | 0.41              |
| 47:2m:1387:G:H2'   | 47:2m:1388:A:O4'   | 2.21                     | 0.41              |
| 47:2m:1689:C:H2'   | 47:2m:1690:U:C6    | 2.54                     | 0.41              |
| 47:2m:1716:C:H2'   | 47:2m:1717:C:H6    | 1.84                     | 0.41              |
| 47:2m:1774:C:H2'   | 47:2m:1775:U:O4'   | 2.21                     | 0.41              |
| 49:2o:62:LEU:HA    | 49:2o:65:ARG:HE    | 1.84                     | 0.41              |
| 50:2p:123:LEU:HD13 | 50:2p:123:LEU:C    | 2.46                     | 0.41              |
| 50:2p:167:TYR:CZ   | 50:2p:204:LEU:HD12 | 2.55                     | 0.41              |
| 51:2q:46:ILE:HG13  | 51:2q:47:PHE:N     | 2.36                     | 0.41              |
| 51:2q:137:PRO:HG3  | 70:3H:209:TYR:CE2  | 2.55                     | 0.41              |
| 53:2s:8:ILE:HD12   | 53:2s:9:VAL:HG22   | 2.01                     | 0.41              |
| 53:2s:181:THR:HG21 | 53:2s:183:LYS:HD2  | 2.03                     | 0.41              |
| 55:2u:11:ILE:HG13  | 55:2u:45:VAL:HG12  | 2.02                     | 0.41              |
| 57:2w:93:MET:SD    | 57:2w:93:MET:C     | 3.03                     | 0.41              |
| 59:2y:66:VAL:HG22  | 59:2y:67:ARG:HG2   | 2.02                     | 0.41              |
| 65:3C:87:ARG:HG2   | 65:3C:91:ALA:CB    | 2.50                     | 0.41              |
| 67:3E:13:LYS:O     | 67:3E:14:PHE:C     | 2.64                     | 0.41              |
| 68:3F:150:TRP:HE3  | 68:3F:170:TRP:CZ3  | 2.39                     | 0.41              |
| 69:3G:82:TYR:OH    | 69:3G:162:ILE:HG23 | 2.20                     | 0.41              |
| 69:3G:172:ASN:O    | 69:3G:174:ILE:N    | 2.52                     | 0.41              |
| 69:3G:205:VAL:HG21 | 69:3G:223:TYR:CD1  | 2.54                     | 0.41              |
| 70:3H:25:ARG:O     | 70:3H:25:ARG:HG3   | 2.20                     | 0.41              |
| 76:3N:99:LYS:HB3   | 76:3N:101:LYS:HZ3  | 1.85                     | 0.41              |
| 77:3O:47:LEU:HB3   | 77:3O:80:ARG:N     | 2.35                     | 0.41              |
| 1:1A:316:U:H3'     | 1:1A:316:U:OP1     | 2.21                     | 0.41              |
| 1:1A:1096:C:H2'    | 1:1A:1097:C:H6     | 1.86                     | 0.41              |
| 1:1A:1836:G:H2'    | 1:1A:1836:G:N3     | 2.36                     | 0.41              |
| 1:1A:2096:G:N3     | 1:1A:2096:G:C2'    | 2.82                     | 0.41              |
| 1:1A:2468:U:O2'    | 1:1A:2506:G:N2     | 2.51                     | 0.41              |
| 1:1A:2481:G:H2'    | 1:1A:2482:C:H6     | 1.80                     | 0.41              |
| 1:1A:2639:U:H2'    | 1:1A:2694:G:C6     | 2.55                     | 0.41              |
| 1:1A:2787:A:N3     | 1:1A:2787:A:C2'    | 2.83                     | 0.41              |
| 1:1A:3690:U:H2'    | 1:1A:3691:G:O4'    | 2.20                     | 0.41              |
| 1:1A:3970:G:H2'    | 1:1A:3971:G:H8     | 1.84                     | 0.41              |
| 1:1A:4108:G:H3'    | 1:1A:4109:G:N7     | 2.36                     | 0.41              |
| 1:1A:4276:G:OP2    | 81:1A:5119:84D:N3  | 2.53                     | 0.41              |
| 1:1A:4428:A:C2'    | 1:1A:4429:C:H5'    | 2.50                     | 0.41              |
| 1:1A:4650:G:H2'    | 1:1A:4651:A:O4'    | 2.21                     | 0.41              |
| 1:1A:4657:U:H3'    | 1:1A:4658:G:H5''   | 2.02                     | 0.41              |
| 1:1A:4950:U:O2     | 1:1A:4950:U:O4'    | 2.39                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:106:G:C2      | 2:1B:107:G:C8      | 3.09                     | 0.41              |
| 3:1C:18:U:C2       | 3:1C:19:C:C5       | 3.08                     | 0.41              |
| 3:1C:82:A:H5'      | 3:1C:83:C:H5''     | 2.03                     | 0.41              |
| 3:1C:92:U:O2'      | 3:1C:93:C:H5'      | 2.21                     | 0.41              |
| 7:1G:213:GLU:OE1   | 7:1G:213:GLU:C     | 2.64                     | 0.41              |
| 8:1H:182:ASN:O     | 8:1H:183:ARG:HB2   | 2.20                     | 0.41              |
| 10:2B:33:GLU:HG3   | 10:2B:34:LYS:N     | 2.36                     | 0.41              |
| 11:2C:43:VAL:HG21  | 11:2C:73:ILE:HD13  | 2.03                     | 0.41              |
| 13:2E:8:LYS:O      | 13:2E:11:PRO:HD2   | 2.20                     | 0.41              |
| 16:2H:184:ILE:HG23 | 16:2H:194:ARG:NH2  | 2.36                     | 0.41              |
| 17:2I:186:GLU:C    | 17:2I:186:GLU:CD   | 2.88                     | 0.41              |
| 20:2L:168:GLU:CD   | 20:2L:172:ARG:HE   | 2.28                     | 0.41              |
| 20:2L:172:ARG:NH1  | 47:2m:908:A:O3'    | 2.33                     | 0.41              |
| 23:2O:23:LEU:HD13  | 23:2O:39:PHE:HE2   | 1.85                     | 0.41              |
| 24:2P:90:ARG:HH11  | 24:2P:96:LEU:HD22  | 1.85                     | 0.41              |
| 28:2T:115:LYS:O    | 28:2T:119:GLU:HG3  | 2.21                     | 0.41              |
| 31:2W:20:LEU:HG    | 31:2W:101:ASP:HB3  | 2.03                     | 0.41              |
| 32:2X:54:MET:HG3   | 32:2X:60:PRO:HA    | 2.03                     | 0.41              |
| 43:2i:23:VAL:HG22  | 43:2i:70:LEU:HD23  | 2.03                     | 0.41              |
| 46:2l:179:LEU:HD23 | 46:2l:182:ASN:HD22 | 1.85                     | 0.41              |
| 47:2m:224:A:H2     | 47:2m:298:G:H1     | 1.68                     | 0.41              |
| 47:2m:321:C:C3'    | 47:2m:322:C:C6     | 3.02                     | 0.41              |
| 47:2m:418:A:O2'    | 47:2m:419:G:OP1    | 2.37                     | 0.41              |
| 47:2m:458:A:H2'    | 47:2m:459:C:H6     | 1.85                     | 0.41              |
| 47:2m:483:C:H2'    | 47:2m:484:A:O4'    | 2.20                     | 0.41              |
| 47:2m:538:U:H1'    | 47:2m:544:G:C6     | 2.56                     | 0.41              |
| 47:2m:562:U:H4'    | 47:2m:562:U:OP1    | 2.21                     | 0.41              |
| 47:2m:839:C:H5'    | 47:2m:840:C:OP2    | 2.21                     | 0.41              |
| 47:2m:878:G:N3     | 47:2m:878:G:C2'    | 2.84                     | 0.41              |
| 47:2m:1380:C:H2'   | 47:2m:1381:G:C1'   | 2.50                     | 0.41              |
| 47:2m:1732:G:H2'   | 47:2m:1733:U:C6    | 2.55                     | 0.41              |
| 47:2m:1780:G:C2'   | 47:2m:1781:A:O5'   | 2.69                     | 0.41              |
| 56:2v:25:LEU:HD22  | 56:2v:25:LEU:N     | 2.31                     | 0.41              |
| 56:2v:60:CYS:CB    | 56:2v:114:SER:HG   | 2.34                     | 0.41              |
| 58:2x:73:LYS:HB3   | 58:2x:73:LYS:HE3   | 1.82                     | 0.41              |
| 60:2z:12:ILE:CD1   | 60:2z:19:ASN:HB2   | 2.49                     | 0.41              |
| 68:3F:149:GLU:HB2  | 68:3F:171:ASP:N    | 2.35                     | 0.41              |
| 68:3F:220:ASP:HB2  | 68:3F:227:LEU:HD23 | 2.02                     | 0.41              |
| 78:3P:8:LEU:HD12   | 78:3P:9:HIS:CE1    | 2.55                     | 0.41              |
| 80:3R:140:TYR:HB2  | 80:3R:147:THR:HB   | 2.01                     | 0.41              |
| 1:1A:180:C:C2'     | 1:1A:181:C:O4'     | 2.68                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:318:A:O2'     | 1:1A:3727:A:H1'   | 2.21                     | 0.41              |
| 1:1A:347:A:OP2     | 27:2S:8:THR:OG1   | 2.31                     | 0.41              |
| 1:1A:456:C:OP2     | 1:1A:456:C:H6     | 2.03                     | 0.41              |
| 1:1A:701:G:H2'     | 1:1A:702:U:C6     | 2.56                     | 0.41              |
| 1:1A:716:C:O2'     | 1:1A:717:U:H5'    | 2.21                     | 0.41              |
| 1:1A:1317:U:OP2    | 33:2Y:40:GLY:HA2  | 2.21                     | 0.41              |
| 1:1A:1355:G:H2'    | 1:1A:1356:U:H6    | 1.80                     | 0.41              |
| 1:1A:1515:A:H2'    | 1:1A:1516:G:O4'   | 2.20                     | 0.41              |
| 1:1A:1686:C:O2     | 1:1A:1686:C:H2'   | 2.21                     | 0.41              |
| 1:1A:1873:A:H5'    | 30:2V:7:HIS:O     | 2.20                     | 0.41              |
| 1:1A:2384:U:H2'    | 1:1A:2385:U:C6    | 2.56                     | 0.41              |
| 1:1A:2563:C:H5''   | 1:1A:2564:G:C8    | 2.55                     | 0.41              |
| 1:1A:2776:G:H2'    | 1:1A:2777:G:C8    | 2.56                     | 0.41              |
| 1:1A:3636:C:H4'    | 1:1A:3825:A:H2    | 1.85                     | 0.41              |
| 1:1A:4187:G:C4'    | 16:2H:82:GLY:HA2  | 2.50                     | 0.41              |
| 1:1A:4200:G:C6     | 1:1A:4201:G:C5    | 3.08                     | 0.41              |
| 2:1B:33:U:O2'      | 2:1B:34:C:H5'     | 2.21                     | 0.41              |
| 2:1B:59:G:C4       | 2:1B:60:G:C8      | 3.09                     | 0.41              |
| 3:1C:65:A:C4       | 3:1C:66:A:C8      | 3.09                     | 0.41              |
| 4:1D:196:TRP:CB    | 4:1D:197:PRO:HD3  | 2.47                     | 0.41              |
| 5:1E:325:GLU:O     | 5:1E:325:GLU:HG3  | 2.20                     | 0.41              |
| 7:1G:23:ARG:O      | 7:1G:23:ARG:HD2   | 2.21                     | 0.41              |
| 7:1G:163:LEU:HD13  | 7:1G:173:ILE:HG21 | 2.02                     | 0.41              |
| 8:1H:128:HIS:O     | 8:1H:128:HIS:CG   | 2.74                     | 0.41              |
| 13:2E:35:ARG:HB3   | 13:2E:126:TYR:HE2 | 1.86                     | 0.41              |
| 14:2F:145:LYS:C    | 14:2F:145:LYS:CD  | 2.94                     | 0.41              |
| 14:2F:146:LEU:HD12 | 14:2F:146:LEU:N   | 2.35                     | 0.41              |
| 19:2K:64:SER:HB3   | 19:2K:92:VAL:CG1  | 2.51                     | 0.41              |
| 20:2L:95:TRP:CD2   | 20:2L:99:MET:HE3  | 2.55                     | 0.41              |
| 21:2M:28:TYR:CD2   | 21:2M:54:MET:HE1  | 2.55                     | 0.41              |
| 22:2N:80:VAL:O     | 22:2N:80:VAL:HG23 | 2.20                     | 0.41              |
| 22:2N:127:GLN:OE1  | 22:2N:127:GLN:HA  | 2.19                     | 0.41              |
| 22:2N:158:PHE:CD1  | 22:2N:158:PHE:C   | 2.98                     | 0.41              |
| 25:2Q:74:ARG:CZ    | 47:2m:1748:G:H5'  | 2.50                     | 0.41              |
| 35:2a:15:THR:O     | 35:2a:19:LYS:HE2  | 2.21                     | 0.41              |
| 46:2l:14:VAL:HG23  | 46:2l:15:ARG:N    | 2.35                     | 0.41              |
| 46:2l:110:PHE:HE2  | 46:2l:133:LYS:CD  | 2.33                     | 0.41              |
| 47:2m:589:G:N2     | 47:2m:591:U:H3    | 2.16                     | 0.41              |
| 47:2m:594:A:C4'    | 47:2m:595:U:H5'   | 2.49                     | 0.41              |
| 47:2m:648:A:H4'    | 64:3B:104:GLY:O   | 2.20                     | 0.41              |
| 47:2m:903:A:O2'    | 47:2m:904:A:H5''  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:1052:A:H2'   | 47:2m:1053:C:O4'   | 2.20                     | 0.41              |
| 47:2m:1114:U:OP2   | 47:2m:1114:U:H3'   | 2.20                     | 0.41              |
| 47:2m:1153:C:O2'   | 47:2m:1154:U:OP2   | 2.31                     | 0.41              |
| 47:2m:1365:G:H2'   | 47:2m:1366:G:H8    | 1.85                     | 0.41              |
| 47:2m:1689:C:H2'   | 47:2m:1690:U:H6    | 1.85                     | 0.41              |
| 47:2m:1777:G:H2'   | 47:2m:1778:C:C6    | 2.56                     | 0.41              |
| 47:2m:1834:A:H2    | 47:2m:1837:G:N1    | 2.18                     | 0.41              |
| 50:2p:21:LEU:HD12  | 50:2p:21:LEU:C     | 2.46                     | 0.41              |
| 50:2p:109:LEU:CD1  | 50:2p:177:LEU:HD12 | 2.50                     | 0.41              |
| 50:2p:162:ASP:N    | 50:2p:163:PRO:HD2  | 2.36                     | 0.41              |
| 51:2q:128:LYS:HG2  | 51:2q:130:PHE:HD1  | 1.86                     | 0.41              |
| 51:2q:138:HIS:CD2  | 51:2q:148:ARG:HG2  | 2.56                     | 0.41              |
| 52:2r:56:TYR:CD2   | 52:2r:66:CYS:HB2   | 2.56                     | 0.41              |
| 53:2s:132:ASP:OD1  | 53:2s:132:ASP:C    | 2.64                     | 0.41              |
| 54:2t:129:LEU:HD12 | 54:2t:133:GLU:CD   | 2.46                     | 0.41              |
| 58:2x:93:VAL:HA    | 58:2x:108:ILE:HD11 | 2.02                     | 0.41              |
| 61:20:130:ASP:HA   | 61:20:133:ARG:CG   | 2.50                     | 0.41              |
| 62:21:46:LYS:HE3   | 62:21:101:ILE:HD11 | 2.01                     | 0.41              |
| 68:3F:116:ASP:HB3  | 68:3F:118:ARG:NE   | 2.35                     | 0.41              |
| 69:3G:74:LYS:HZ3   | 69:3G:272:HIS:HB2  | 1.85                     | 0.41              |
| 71:3I:121:LYS:H    | 71:3I:121:LYS:HD2  | 1.86                     | 0.41              |
| 71:3I:132:GLN:HB2  | 71:3I:134:HIS:CD2  | 2.55                     | 0.41              |
| 76:3N:10:ARG:NH1   | 76:3N:70:THR:HG23  | 2.35                     | 0.41              |
| 76:3N:14:THR:HB    | 76:3N:21:LYS:HG2   | 2.01                     | 0.41              |
| 76:3N:84:LYS:HE3   | 76:3N:84:LYS:HB3   | 1.78                     | 0.41              |
| 76:3N:109:GLU:HG2  | 76:3N:110:ARG:N    | 2.34                     | 0.41              |
| 77:3O:58:LEU:HD22  | 77:3O:62:VAL:HG21  | 2.03                     | 0.41              |
| 79:3Q:13:ARG:O     | 79:3Q:16:THR:HG22  | 2.21                     | 0.41              |
| 1:1A:66:A:O2'      | 1:1A:67:C:OP2      | 2.34                     | 0.41              |
| 1:1A:121:A:OP1     | 10:2B:110:LYS:HE3  | 2.21                     | 0.41              |
| 1:1A:1086:C:C2'    | 1:1A:1087:A:H5'    | 2.51                     | 0.41              |
| 1:1A:1337:A:H5''   | 6:1F:102:PHE:CD2   | 2.55                     | 0.41              |
| 1:1A:1601:A:H3'    | 38:2d:2:THR:HG21   | 2.02                     | 0.41              |
| 1:1A:1632:A:N3     | 1:1A:1632:A:C2'    | 2.84                     | 0.41              |
| 1:1A:1687:U:H2'    | 1:1A:1688:G:C8     | 2.56                     | 0.41              |
| 1:1A:1770:A:H2'    | 1:1A:1771:U:O4'    | 2.20                     | 0.41              |
| 1:1A:1978:C:N4     | 1:1A:1979:A:N3     | 2.68                     | 0.41              |
| 1:1A:2083:C:P      | 19:2K:14:ARG:HH22  | 2.41                     | 0.41              |
| 1:1A:2517:A:H5'    | 35:2a:62:LYS:CE    | 2.50                     | 0.41              |
| 1:1A:2616:C:OP1    | 20:2L:64:ARG:HD3   | 2.21                     | 0.41              |
| 1:1A:2627:C:O2     | 1:1A:2627:C:H2'    | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1A:2801:U:OP2    | 81:1A:5107:84D:N2 | 2.54                     | 0.41              |
| 1:1A:2907:G:H1'    | 1:1A:3589:G:N1    | 2.17                     | 0.41              |
| 1:1A:3676:G:O2'    | 1:1A:3677:U:H5'   | 2.20                     | 0.41              |
| 1:1A:3807:A:OP1    | 42:2h:23:ARG:NH1  | 2.49                     | 0.41              |
| 1:1A:3962:A:H1'    | 1:1A:3963:A:H5''  | 2.03                     | 0.41              |
| 1:1A:3974:G:H22    | 1:1A:4050:A:H8    | 1.69                     | 0.41              |
| 1:1A:4082:G:H2'    | 1:1A:4083:U:C2    | 2.56                     | 0.41              |
| 1:1A:4103:C:C2'    | 1:1A:4104:G:H5''  | 2.51                     | 0.41              |
| 1:1A:4199:C:C4     | 1:1A:4200:G:C8    | 3.09                     | 0.41              |
| 1:1A:4247:G:C2'    | 1:1A:4248:A:H5'   | 2.51                     | 0.41              |
| 1:1A:4364:G:O4'    | 29:2U:58:MET:HG2  | 2.20                     | 0.41              |
| 1:1A:4551:U:H2'    | 1:1A:4552:U:C6    | 2.55                     | 0.41              |
| 1:1A:5055:G:H2'    | 1:1A:5056:A:H8    | 1.86                     | 0.41              |
| 3:1C:67:U:OP1      | 38:2d:87:LYS:HG3  | 2.21                     | 0.41              |
| 3:1C:132:G:N3      | 3:1C:133:G:C8     | 2.89                     | 0.41              |
| 5:1E:148:LYS:HE3   | 5:1E:148:LYS:HB2  | 1.86                     | 0.41              |
| 9:2A:209:TRP:CD1   | 9:2A:210:PRO:HD2  | 2.56                     | 0.41              |
| 10:2B:120:LYS:HB3  | 10:2B:125:LYS:HG2 | 2.02                     | 0.41              |
| 10:2B:125:LYS:HE2  | 10:2B:128:VAL:CB  | 2.50                     | 0.41              |
| 13:2E:32:ARG:CG    | 13:2E:126:TYR:HE1 | 2.33                     | 0.41              |
| 16:2H:83:LYS:O     | 16:2H:85:VAL:N    | 2.53                     | 0.41              |
| 19:2K:50:ARG:HA    | 19:2K:53:MET:CG   | 2.36                     | 0.41              |
| 20:2L:168:GLU:OE1  | 20:2L:172:ARG:NE  | 2.47                     | 0.41              |
| 23:2O:19:LEU:HB3   | 23:2O:74:SER:C    | 2.40                     | 0.41              |
| 23:2O:33:ILE:HG13  | 23:2O:33:ILE:O    | 2.21                     | 0.41              |
| 26:2R:147:LEU:HD22 | 26:2R:147:LEU:HA  | 1.89                     | 0.41              |
| 28:2T:10:VAL:O     | 28:2T:83:THR:OG1  | 2.29                     | 0.41              |
| 28:2T:12:LEU:HB2   | 28:2T:81:MET:HB3  | 2.03                     | 0.41              |
| 28:2T:87:VAL:HG22  | 28:2T:89:ILE:HG23 | 2.03                     | 0.41              |
| 46:2l:48:ARG:NH1   | 46:2l:50:SER:HB3  | 2.36                     | 0.41              |
| 46:2l:65:VAL:HG12  | 46:2l:111:LEU:HA  | 2.03                     | 0.41              |
| 47:2m:164:A:OP1    | 70:3H:83:CYS:N    | 2.52                     | 0.41              |
| 47:2m:353:C:H2'    | 47:2m:354:U:C6    | 2.55                     | 0.41              |
| 47:2m:1056:U:O2'   | 47:2m:1057:C:H5'  | 2.21                     | 0.41              |
| 47:2m:1265:A:N3    | 47:2m:1265:A:C2'  | 2.83                     | 0.41              |
| 47:2m:1266:C:H42   | 47:2m:1517:G:H22  | 1.69                     | 0.41              |
| 47:2m:1650:A:H2    | 52:2r:83:ASN:HD22 | 1.68                     | 0.41              |
| 47:2m:1656:G:C5    | 47:2m:1669:G:C2   | 3.09                     | 0.41              |
| 47:2m:1688:C:H2'   | 47:2m:1689:C:H6   | 1.85                     | 0.41              |
| 47:2m:1865:C:C6    | 65:3C:92:ARG:HB3  | 2.56                     | 0.41              |
| 53:2s:7:LYS:NZ     | 53:2s:24:SER:H    | 2.18                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:2s:20:GLU:HA    | 53:2s:23:ILE:HG13  | 2.02                     | 0.41              |
| 53:2s:49:LYS:HD2   | 53:2s:179:LYS:HZ2  | 1.86                     | 0.41              |
| 54:2t:143:LYS:HA   | 54:2t:146:GLN:CG   | 2.51                     | 0.41              |
| 56:2v:61:PRO:HD3   | 56:2v:141:ASN:CG   | 2.46                     | 0.41              |
| 58:2x:27:ARG:HA    | 58:2x:27:ARG:HE    | 1.85                     | 0.41              |
| 58:2x:92:LEU:HD11  | 58:2x:108:ILE:HD12 | 2.03                     | 0.41              |
| 60:2z:19:ASN:O     | 60:2z:19:ASN:ND2   | 2.52                     | 0.41              |
| 60:2z:22:GLY:HA2   | 60:2z:56:ALA:HB3   | 2.03                     | 0.41              |
| 68:3F:8:ARG:HD2    | 68:3F:8:ARG:O      | 2.21                     | 0.41              |
| 70:3H:114:VAL:HG13 | 70:3H:115:LYS:N    | 2.35                     | 0.41              |
| 77:3O:47:LEU:CD1   | 77:3O:50:PHE:HB3   | 2.51                     | 0.41              |
| 1:1A:33:A:H3'      | 1:1A:47:A:H61      | 1.85                     | 0.41              |
| 1:1A:121:A:N3      | 1:1A:121:A:H2'     | 2.36                     | 0.41              |
| 1:1A:124:C:H2'     | 1:1A:125:C:H6      | 1.85                     | 0.41              |
| 1:1A:146:G:O2'     | 1:1A:147:A:H5'     | 2.21                     | 0.41              |
| 1:1A:336:A:H5''    | 1:1A:337:U:OP2     | 2.21                     | 0.41              |
| 1:1A:414:C:H5'     | 1:1A:415:G:OP2     | 2.20                     | 0.41              |
| 1:1A:441:G:H2'     | 1:1A:442:G:H8      | 1.86                     | 0.41              |
| 1:1A:740:G:C8      | 1:1A:741:C:H5      | 2.39                     | 0.41              |
| 1:1A:743:G:H5''    | 1:1A:744:G:OP2     | 2.21                     | 0.41              |
| 1:1A:979:C:OP2     | 8:1H:66:LYS:HD2    | 2.20                     | 0.41              |
| 1:1A:1249:C:H2'    | 1:1A:1250:C:H6     | 1.86                     | 0.41              |
| 1:1A:1370:G:O6     | 6:1F:239:LYS:HE3   | 2.20                     | 0.41              |
| 1:1A:1417:C:H2'    | 1:1A:1418:C:C6     | 2.56                     | 0.41              |
| 1:1A:1478:C:O2'    | 1:1A:1479:G:H5'    | 2.21                     | 0.41              |
| 1:1A:1527:A:H2'    | 1:1A:1528:U:C6     | 2.56                     | 0.41              |
| 1:1A:1898:C:O2'    | 1:1A:2279:A:H5'    | 2.21                     | 0.41              |
| 1:1A:1919:G:O2'    | 34:2Z:81:SER:HB3   | 2.21                     | 0.41              |
| 1:1A:2005:G:H22    | 1:1A:2014:C:H42    | 1.68                     | 0.41              |
| 1:1A:2480:G:H2'    | 1:1A:2481:G:H8     | 1.86                     | 0.41              |
| 1:1A:2563:C:H5'    | 1:1A:2564:G:OP2    | 2.20                     | 0.41              |
| 1:1A:2695:A:C5'    | 1:1A:2696:A:H8     | 2.34                     | 0.41              |
| 1:1A:2752:G:H2'    | 1:1A:2753:G:H8     | 1.85                     | 0.41              |
| 1:1A:2762:G:H1'    | 1:1A:2763:U:O4'    | 2.21                     | 0.41              |
| 1:1A:3616:U:C4'    | 1:1A:3617:G:H5'    | 2.37                     | 0.41              |
| 1:1A:3652:A:C3'    | 1:1A:3653:A:C8     | 3.03                     | 0.41              |
| 1:1A:3654:G:N2     | 1:1A:3817:A:H2     | 2.19                     | 0.41              |
| 1:1A:3670:C:O2'    | 1:1A:3671:G:P      | 2.79                     | 0.41              |
| 1:1A:3672:G:H8     | 1:1A:3672:G:O5'    | 2.04                     | 0.41              |
| 1:1A:3692:A:C4     | 1:1A:3693:U:C6     | 3.09                     | 0.41              |
| 1:1A:3746:A:H5''   | 4:1D:244:GLY:HA3   | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:3773:U:C5'    | 1:1A:3774:A:H3'    | 2.50                     | 0.41              |
| 1:1A:3882:C:O2     | 1:1A:3882:C:H2'    | 2.20                     | 0.41              |
| 1:1A:4499:G:H1'    | 1:1A:4528:G:N3     | 2.35                     | 0.41              |
| 1:1A:4524:G:N3     | 5:1E:252:ALA:HB1   | 2.36                     | 0.41              |
| 1:1A:4758:U:H2'    | 1:1A:4759:C:O4'    | 2.21                     | 0.41              |
| 1:1A:4915:G:O2'    | 1:1A:4916:G:H5'    | 2.20                     | 0.41              |
| 1:1A:5066:U:H2'    | 1:1A:5067:U:C6     | 2.56                     | 0.41              |
| 2:1B:38:U:N3       | 2:1B:41:G:OP2      | 2.33                     | 0.41              |
| 2:1B:106:G:N3      | 2:1B:107:G:C8      | 2.89                     | 0.41              |
| 3:1C:47:C:O2'      | 3:1C:62:A:OP2      | 2.35                     | 0.41              |
| 3:1C:68:G:O2'      | 3:1C:69:U:H5'      | 2.21                     | 0.41              |
| 3:1C:132:G:O2'     | 3:1C:133:G:H5'     | 2.21                     | 0.41              |
| 7:1G:39:GLN:HG3    | 7:1G:40:ASP:N      | 2.36                     | 0.41              |
| 7:1G:288:LEU:HD23  | 7:1G:288:LEU:HA    | 1.86                     | 0.41              |
| 8:1H:206:VAL:HG12  | 8:1H:208:ILE:HD12  | 2.03                     | 0.41              |
| 8:1H:245:GLN:O     | 8:1H:249:ASP:OD2   | 2.39                     | 0.41              |
| 9:2A:124:LYS:HD3   | 9:2A:197:VAL:HG11  | 2.03                     | 0.41              |
| 11:2C:91:LYS:HB2   | 11:2C:183:GLU:HG3  | 2.03                     | 0.41              |
| 11:2C:118:LEU:HD11 | 11:2C:167:VAL:CG2  | 2.37                     | 0.41              |
| 13:2E:18:ARG:HG3   | 13:2E:135:GLY:HA3  | 2.03                     | 0.41              |
| 13:2E:88:LYS:HA    | 13:2E:92:TYR:CE1   | 2.56                     | 0.41              |
| 15:2G:50:MET:HE3   | 15:2G:50:MET:HB2   | 1.96                     | 0.41              |
| 15:2G:71:LYS:HB2   | 15:2G:71:LYS:HE3   | 1.82                     | 0.41              |
| 15:2G:108:ASP:OD1  | 15:2G:108:ASP:N    | 2.54                     | 0.41              |
| 16:2H:27:CYS:SG    | 16:2H:124:ASP:HB2  | 2.60                     | 0.41              |
| 18:2J:36:ILE:CD1   | 18:2J:47:TYR:HD2   | 2.31                     | 0.41              |
| 18:2J:140:MET:HE3  | 18:2J:140:MET:HB3  | 1.99                     | 0.41              |
| 19:2K:159:PRO:HA   | 19:2K:188:ASN:OXT  | 2.21                     | 0.41              |
| 20:2L:78:ILE:HD12  | 20:2L:78:ILE:HA    | 1.88                     | 0.41              |
| 21:2M:75:VAL:HG11  | 21:2M:98:ARG:NH2   | 2.35                     | 0.41              |
| 24:2P:45:ILE:HG21  | 24:2P:53:PRO:HB3   | 2.03                     | 0.41              |
| 32:2X:22:THR:CG2   | 32:2X:122:VAL:HB   | 2.46                     | 0.41              |
| 33:2Y:28:TYR:HB2   | 33:2Y:31:ILE:HG12  | 2.02                     | 0.41              |
| 34:2Z:45:LYS:HE3   | 34:2Z:105:LEU:HD12 | 2.03                     | 0.41              |
| 40:2f:33:ASN:ND2   | 40:2f:35:ILE:O     | 2.54                     | 0.41              |
| 43:2i:93:LEU:HD12  | 43:2i:93:LEU:HA    | 1.81                     | 0.41              |
| 44:2j:36:LYS:HE2   | 44:2j:36:LYS:HB2   | 1.72                     | 0.41              |
| 45:2k:64:ILE:HG23  | 45:2k:102:TYR:CZ   | 2.55                     | 0.41              |
| 46:2l:68:LEU:HD22  | 46:2l:83:PRO:C     | 2.46                     | 0.41              |
| 47:2m:66:G:OP1     | 70:3H:172:LYS:NZ   | 2.39                     | 0.41              |
| 47:2m:301:A:C2'    | 54:2t:73:THR:HG22  | 2.51                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:2m:527:C:OP1    | 71:3I:122:SER:OG   | 2.38                     | 0.41              |
| 47:2m:630:U:O2     | 47:2m:630:U:C2'    | 2.69                     | 0.41              |
| 47:2m:681:U:O2'    | 47:2m:1160:U:OP1   | 2.37                     | 0.41              |
| 47:2m:690:G:O2'    | 47:2m:691:G:H5''   | 2.21                     | 0.41              |
| 47:2m:798:A:H5'    | 47:2m:799:U:O3'    | 2.21                     | 0.41              |
| 47:2m:881:G:O5'    | 47:2m:881:G:H8     | 2.04                     | 0.41              |
| 47:2m:1047:C:H5''  | 74:3L:143:LYS:CB   | 2.23                     | 0.41              |
| 47:2m:1069:U:H2'   | 47:2m:1070:A:C8    | 2.56                     | 0.41              |
| 47:2m:1159:G:H2'   | 47:2m:1160:U:O4'   | 2.21                     | 0.41              |
| 47:2m:1189:A:OP1   | 64:3B:28:LYS:HD3   | 2.21                     | 0.41              |
| 47:2m:1223:A:H3'   | 47:2m:1224:G:H5''  | 2.03                     | 0.41              |
| 47:2m:1283:C:H5'   | 47:2m:1284:A:OP2   | 2.21                     | 0.41              |
| 47:2m:1294:G:H8    | 47:2m:1294:G:OP2   | 2.04                     | 0.41              |
| 47:2m:1297:U:N3    | 47:2m:1300:U:OP2   | 2.51                     | 0.41              |
| 47:2m:1309:C:H41   | 80:3R:100:LEU:HD11 | 1.85                     | 0.41              |
| 47:2m:1349:G:H2'   | 47:2m:1350:U:C6    | 2.56                     | 0.41              |
| 47:2m:1384:C:H5''  | 50:2p:157:MET:O    | 2.21                     | 0.41              |
| 47:2m:1438:A:H62   | 47:2m:1439:A:N6    | 2.19                     | 0.41              |
| 47:2m:1495:G:H2'   | 47:2m:1496:U:O5'   | 2.21                     | 0.41              |
| 47:2m:1532:C:O4'   | 47:2m:1604:G:N2    | 2.54                     | 0.41              |
| 47:2m:1538:C:O2'   | 47:2m:1539:U:O5'   | 2.34                     | 0.41              |
| 47:2m:1542:C:HO2'  | 47:2m:1543:U:P     | 2.42                     | 0.41              |
| 47:2m:1605:G:H3'   | 47:2m:1606:G:C8    | 2.55                     | 0.41              |
| 47:2m:1606:G:H5''  | 61:20:86:GLY:HA3   | 2.03                     | 0.41              |
| 47:2m:1648:G:H5''  | 58:2x:125:ARG:CG   | 2.51                     | 0.41              |
| 47:2m:1654:G:H2'   | 47:2m:1655:C:H6    | 1.86                     | 0.41              |
| 47:2m:1656:G:H2'   | 47:2m:1656:G:N3    | 2.36                     | 0.41              |
| 47:2m:1733:U:C2'   | 47:2m:1734:G:H5'   | 2.51                     | 0.41              |
| 48:2n:69:GLU:OE1   | 69:3G:270:THR:HG21 | 2.21                     | 0.41              |
| 48:2n:124:VAL:HG13 | 48:2n:130:ASP:OD2  | 2.21                     | 0.41              |
| 48:2n:153:PRO:C    | 48:2n:154:LEU:HD23 | 2.45                     | 0.41              |
| 49:2o:72:ALA:HB2   | 49:2o:80:ALA:HB2   | 2.03                     | 0.41              |
| 49:2o:134:LEU:CG   | 49:2o:218:LEU:HD12 | 2.38                     | 0.41              |
| 49:2o:175:GLU:OE1  | 49:2o:175:GLU:HA   | 2.21                     | 0.41              |
| 49:2o:197:ILE:HB   | 49:2o:210:VAL:HG11 | 2.03                     | 0.41              |
| 49:2o:213:ARG:HG2  | 49:2o:213:ARG:HH11 | 1.86                     | 0.41              |
| 50:2p:75:LYS:HZ3   | 50:2p:75:LYS:HB2   | 1.85                     | 0.41              |
| 51:2q:80:ILE:HG13  | 51:2q:81:THR:HG23  | 2.03                     | 0.41              |
| 52:2r:39:ILE:O     | 52:2r:39:ILE:CG2   | 2.68                     | 0.41              |
| 52:2r:168:THR:OG1  | 52:2r:171:GLU:OE2  | 2.29                     | 0.41              |
| 54:2t:17:LYS:HZ2   | 54:2t:17:LYS:HG3   | 1.74                     | 0.41              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 56:2v:45:LYS:H     | 56:2v:45:LYS:HG2     | 1.53                     | 0.41              |
| 56:2v:126:VAL:HG22 | 56:2v:145:VAL:HG22   | 2.02                     | 0.41              |
| 57:2w:108:LYS:HD2  | 57:2w:110:GLU:HB2    | 2.03                     | 0.41              |
| 58:2x:54:PRO:HG2   | 58:2x:88:ILE:CD1     | 2.45                     | 0.41              |
| 59:2y:11:LYS:HG3   | 59:2y:12:ALA:N       | 2.34                     | 0.41              |
| 61:20:28:LEU:HB3   | 61:20:110:LEU:HD11   | 2.02                     | 0.41              |
| 63:3A:82:ASN:O     | 63:3A:82:ASN:ND2     | 2.53                     | 0.41              |
| 64:3B:36:LEU:O     | 64:3B:36:LEU:HD22    | 2.20                     | 0.41              |
| 65:3C:58:VAL:CG1   | 74:3L:125:LYS:HB3    | 2.51                     | 0.41              |
| 65:3C:82:LYS:HG2   | 65:3C:85[A]:ARG:HH11 | 1.86                     | 0.41              |
| 68:3F:127:LYS:HD2  | 68:3F:148:SER:HA     | 2.01                     | 0.41              |
| 68:3F:152:SER:HB2  | 68:3F:169:GLY:HA2    | 2.03                     | 0.41              |
| 69:3G:65:LYS:O     | 69:3G:69:LEU:HG      | 2.20                     | 0.41              |
| 69:3G:79:GLU:OE1   | 69:3G:80:GLU:N       | 2.53                     | 0.41              |
| 71:3I:60:LEU:HB3   | 71:3I:94:LEU:HD21    | 2.03                     | 0.41              |
| 71:3I:138[A]:ARG:H | 71:3I:138[A]:ARG:HG3 | 1.41                     | 0.41              |
| 74:3L:61:LYS:HD2   | 74:3L:61:LYS:HA      | 1.87                     | 0.41              |
| 74:3L:121:ARG:HA   | 74:3L:121:ARG:HD2    | 1.58                     | 0.41              |
| 75:3M:8:ALA:HA     | 75:3M:74:VAL:HG11    | 2.03                     | 0.41              |
| 75:3M:88:LYS:HD3   | 75:3M:88:LYS:HA      | 1.70                     | 0.41              |
| 76:3N:23:MET:HE2   | 76:3N:23:MET:HB2     | 1.97                     | 0.41              |
| 78:3P:35:VAL:HG11  | 78:3P:46:VAL:HG23    | 2.03                     | 0.41              |
| 1:1A:270:U:C2      | 1:1A:271:C:C5        | 3.09                     | 0.41              |
| 1:1A:362:A:N6      | 40:2f:37:TYR:O       | 2.47                     | 0.41              |
| 1:1A:510:U:OP1     | 14:2F:163:LYS:NZ     | 2.45                     | 0.41              |
| 1:1A:722:G:H2'     | 1:1A:723:A:C8        | 2.56                     | 0.41              |
| 1:1A:1703:C:OP1    | 1:1A:1703:C:H4'      | 2.21                     | 0.41              |
| 1:1A:1937:C:OP2    | 1:1A:1938:C:O2'      | 2.31                     | 0.41              |
| 1:1A:2602:G:H2'    | 1:1A:2603:C:H6       | 1.86                     | 0.41              |
| 1:1A:3690:U:C2'    | 1:1A:3691:G:H5'      | 2.49                     | 0.41              |
| 1:1A:4260:U:O2'    | 13:2E:133:VAL:HG21   | 2.21                     | 0.41              |
| 1:1A:4424:A:N7     | 1:1A:4475:G:C6       | 2.89                     | 0.41              |
| 1:1A:4612:C:H2'    | 1:1A:4613:C:H5'      | 2.03                     | 0.41              |
| 1:1A:4704:C:H2'    | 1:1A:4705:A:H8       | 1.86                     | 0.41              |
| 1:1A:4884:G:N2     | 1:1A:4936:G:H1       | 2.19                     | 0.41              |
| 1:1A:4991:U:H2'    | 1:1A:4992:G:C8       | 2.56                     | 0.41              |
| 3:1C:65:A:H2'      | 3:1C:66:A:H8         | 1.86                     | 0.41              |
| 9:2A:199:LYS:HE3   | 9:2A:199:LYS:HB2     | 1.74                     | 0.41              |
| 11:2C:105:ILE:HG22 | 11:2C:109:GLY:HA2    | 2.02                     | 0.41              |
| 12:2D:91:LEU:HD11  | 12:2D:129:VAL:CG1    | 2.51                     | 0.41              |
| 15:2G:96:GLU:OE1   | 15:2G:100:ARG:NH2    | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:2H:110:CYS:HB3  | 16:2H:113:LEU:HD12 | 2.03                     | 0.41              |
| 21:2M:106:VAL:HG13 | 21:2M:126:ILE:HD13 | 2.03                     | 0.41              |
| 28:2T:48:ARG:HB2   | 28:2T:69:LYS:HB3   | 2.02                     | 0.41              |
| 30:2V:93:LEU:HD23  | 30:2V:93:LEU:HA    | 1.72                     | 0.41              |
| 33:2Y:89:LEU:HD13  | 33:2Y:118:LEU:HD22 | 2.02                     | 0.41              |
| 47:2m:429:C:P      | 71:3I:2:PRO:HD2    | 2.61                     | 0.41              |
| 47:2m:523:A:C2     | 47:2m:524:U:H1'    | 2.56                     | 0.41              |
| 47:2m:681:U:O2'    | 47:2m:682:U:H5'    | 2.21                     | 0.41              |
| 47:2m:738:C:O2     | 47:2m:738:C:C3'    | 2.67                     | 0.41              |
| 47:2m:1189:A:H4'   | 64:3B:34:THR:HG21  | 2.02                     | 0.41              |
| 47:2m:1236:G:C2'   | 47:2m:1237:C:H5'   | 2.51                     | 0.41              |
| 47:2m:1277:C:H2'   | 47:2m:1278:A:C8    | 2.55                     | 0.41              |
| 47:2m:1473:G:H21   | 47:2m:1475:G:C3'   | 2.33                     | 0.41              |
| 47:2m:1523:C:OP2   | 60:2z:141:ARG:HB3  | 2.21                     | 0.41              |
| 47:2m:1535:U:OP2   | 52:2r:168:THR:HB   | 2.21                     | 0.41              |
| 47:2m:1596:U:C4    | 47:2m:1597:C:C5    | 3.09                     | 0.41              |
| 47:2m:1599:U:H4'   | 47:2m:1600:G:C4    | 2.56                     | 0.41              |
| 47:2m:1644:C:OP1   | 58:2x:143:LYS:N    | 2.54                     | 0.41              |
| 49:2o:110:MET:HE3  | 49:2o:110:MET:C    | 2.45                     | 0.41              |
| 53:2s:15:LYS:HA    | 53:2s:15:LYS:HD2   | 1.85                     | 0.41              |
| 54:2t:79:ILE:CD1   | 54:2t:170:LYS:HD3  | 2.30                     | 0.41              |
| 55:2u:52:LEU:CD2   | 55:2u:58:VAL:HG13  | 2.48                     | 0.41              |
| 55:2u:77:GLN:HA    | 55:2u:80:ARG:NH2   | 2.35                     | 0.41              |
| 59:2y:45:LYS:HA    | 59:2y:48:ASN:OD1   | 2.20                     | 0.41              |
| 61:20:29:LYS:HD2   | 61:20:29:LYS:C     | 2.47                     | 0.41              |
| 62:21:48:LEU:CD1   | 62:21:93:SER:HB2   | 2.49                     | 0.41              |
| 62:21:81:GLN:CD    | 67:3E:55:LEU:HB2   | 2.46                     | 0.41              |
| 62:21:96:GLU:OE1   | 62:21:96:GLU:N     | 2.52                     | 0.41              |
| 64:3B:54:LYS:HD3   | 64:3B:91:LEU:CD1   | 2.51                     | 0.41              |
| 68:3F:106:LYS:NZ   | 68:3F:106:LYS:HB3  | 2.36                     | 0.41              |
| 68:3F:178:ASN:HB2  | 68:3F:185:LYS:HG3  | 2.02                     | 0.41              |
| 69:3G:63:VAL:O     | 69:3G:63:VAL:HG13  | 2.22                     | 0.41              |
| 69:3G:183:LYS:HE3  | 69:3G:194:ARG:NH2  | 2.36                     | 0.41              |
| 70:3H:55:GLY:H     | 70:3H:63:MET:HG2   | 1.86                     | 0.41              |
| 70:3H:85:ARG:HG2   | 70:3H:85:ARG:O     | 2.21                     | 0.41              |
| 71:3I:32:ILE:HG12  | 71:3I:37:LEU:HB2   | 2.02                     | 0.41              |
| 71:3I:83:ARG:HH21  | 71:3I:150:ARG:CD   | 2.34                     | 0.41              |
| 75:3M:87:GLU:CD    | 75:3M:88:LYS:H     | 2.28                     | 0.41              |
| 77:3O:62:VAL:N     | 77:3O:63:PRO:CD    | 2.84                     | 0.41              |
| 77:3O:63:PRO:C     | 77:3O:97:ILE:HD11  | 2.46                     | 0.41              |
| 1:1A:100:C:C6      | 1:1A:101:A:C8      | 3.08                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:227:A:C2'     | 1:1A:228:C:H5'     | 2.50                     | 0.40              |
| 1:1A:965:G:C2'     | 1:1A:966:A:OP2     | 2.69                     | 0.40              |
| 1:1A:985:C:H2'     | 1:1A:986:C:H6      | 1.86                     | 0.40              |
| 1:1A:1269:G:O2'    | 1:1A:1440:U:O3'    | 2.39                     | 0.40              |
| 1:1A:1468:C:H2'    | 1:1A:1469:C:H6     | 1.84                     | 0.40              |
| 1:1A:1631:A:C6     | 4:1D:204:MET:HE2   | 2.56                     | 0.40              |
| 1:1A:1947:U:H4'    | 1:1A:1948:G:OP1    | 2.20                     | 0.40              |
| 1:1A:4503:A:O2'    | 1:1A:4504:C:H5'    | 2.20                     | 0.40              |
| 1:1A:4621:C:O2'    | 1:1A:4622:A:H5'    | 2.22                     | 0.40              |
| 1:1A:4902:C:H2'    | 1:1A:4903:G:C8     | 2.52                     | 0.40              |
| 1:1A:5043:A:H2'    | 1:1A:5044:A:C8     | 2.56                     | 0.40              |
| 1:1A:5043:A:H2'    | 1:1A:5044:A:H8     | 1.86                     | 0.40              |
| 3:1C:72:A:P        | 27:2S:51:LYS:HB2   | 2.61                     | 0.40              |
| 3:1C:90:C:H2'      | 3:1C:91:A:C8       | 2.56                     | 0.40              |
| 3:1C:122:G:C5      | 3:1C:123:U:H1'     | 2.56                     | 0.40              |
| 10:2B:156:VAL:HG13 | 10:2B:182:CYS:SG   | 2.61                     | 0.40              |
| 13:2E:13:ARG:N     | 13:2E:14:GLU:OE1   | 2.54                     | 0.40              |
| 13:2E:74:VAL:HG11  | 13:2E:78:LYS:HG3   | 2.04                     | 0.40              |
| 15:2G:25:VAL:HG21  | 15:2G:38:VAL:CG1   | 2.51                     | 0.40              |
| 15:2G:65:PRO:HG2   | 15:2G:68:ALA:HB2   | 2.03                     | 0.40              |
| 18:2J:36:ILE:HA    | 18:2J:36:ILE:HD13  | 1.88                     | 0.40              |
| 19:2K:29:VAL:O     | 19:2K:33:ARG:HB2   | 2.21                     | 0.40              |
| 23:2O:82:TYR:HD1   | 23:2O:82:TYR:O     | 2.03                     | 0.40              |
| 26:2R:73:HIS:CD2   | 26:2R:112:ALA:HA   | 2.57                     | 0.40              |
| 28:2T:103:ASP:CG   | 28:2T:106:LEU:HG   | 2.44                     | 0.40              |
| 47:2m:442:C:C2'    | 47:2m:443:U:H5'    | 2.51                     | 0.40              |
| 47:2m:561:A:C5'    | 71:3I:171:GLY:HA3  | 2.51                     | 0.40              |
| 47:2m:744:G:N3     | 47:2m:744:G:C2'    | 2.82                     | 0.40              |
| 47:2m:921:G:O6     | 75:3M:60:LYS:NZ    | 2.51                     | 0.40              |
| 47:2m:1372:U:O2'   | 47:2m:1373:C:P     | 2.80                     | 0.40              |
| 47:2m:1614:A:C2    | 47:2m:1615:U:C5    | 3.09                     | 0.40              |
| 47:2m:1752:C:H2'   | 47:2m:1753:C:C5'   | 2.41                     | 0.40              |
| 48:2n:83:GLY:O     | 48:2n:87:VAL:HG22  | 2.21                     | 0.40              |
| 50:2p:11:PHE:HD2   | 62:2I:84:ILE:CD1   | 2.34                     | 0.40              |
| 50:2p:116:ARG:HG3  | 50:2p:120:TYR:CE1  | 2.56                     | 0.40              |
| 50:2p:223:ILE:HG23 | 68:3F:189:ILE:HG13 | 2.03                     | 0.40              |
| 51:2q:221:ARG:HG3  | 51:2q:224:ASN:OD1  | 2.22                     | 0.40              |
| 52:2r:40:ALA:HA    | 52:2r:45:TYR:CE1   | 2.55                     | 0.40              |
| 53:2s:46:THR:HB    | 53:2s:63:PHE:O     | 2.21                     | 0.40              |
| 53:2s:98:ARG:HD2   | 53:2s:98:ARG:HA    | 1.41                     | 0.40              |
| 53:2s:100:ILE:HG13 | 53:2s:125:VAL:CG2  | 2.49                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:2u:15:LEU:CD1  | 55:2u:49:MET:HE1  | 2.42                     | 0.40              |
| 55:2u:65:ARG:NH1  | 67:3E:21:CYS:O    | 2.53                     | 0.40              |
| 56:2v:35:ARG:HG2  | 56:2v:51:ILE:O    | 2.22                     | 0.40              |
| 58:2x:12:VAL:HG21 | 58:2x:90:LYS:C    | 2.46                     | 0.40              |
| 59:2y:109:LEU:HG  | 59:2y:109:LEU:O   | 2.22                     | 0.40              |
| 60:2z:80:PRO:HB2  | 60:2z:82:TRP:NE1  | 2.36                     | 0.40              |
| 60:2z:89:ASP:O    | 60:2z:93:GLY:N    | 2.46                     | 0.40              |
| 71:3I:57:ALA:O    | 71:3I:61:LEU:HD23 | 2.20                     | 0.40              |
| 73:3K:99:ARG:NH1  | 73:3K:143:SER:HB2 | 2.36                     | 0.40              |
| 73:3K:132:LYS:O   | 73:3K:133:ARG:HB2 | 2.20                     | 0.40              |
| 76:3N:87:PRO:HG2  | 76:3N:90:ARG:NH2  | 2.36                     | 0.40              |
| 77:3O:68:ILE:HG22 | 77:3O:88:LEU:CD2  | 2.51                     | 0.40              |
| 1:1A:89:C:C2'     | 1:1A:90:G:H5'     | 2.52                     | 0.40              |
| 1:1A:462:G:H2'    | 1:1A:463:A:H8     | 1.80                     | 0.40              |
| 1:1A:490:C:N4     | 1:1A:664:G:O6     | 2.53                     | 0.40              |
| 1:1A:726:G:H2'    | 1:1A:727:C:C6     | 2.56                     | 0.40              |
| 1:1A:750:U:H1'    | 1:1A:917:A:C8     | 2.56                     | 0.40              |
| 1:1A:757:G:C2     | 1:1A:758:G:C8     | 3.10                     | 0.40              |
| 1:1A:1174:G:H22   | 1:1A:1186:U:H3    | 1.69                     | 0.40              |
| 1:1A:1399:G:H2'   | 1:1A:1400:G:H8    | 1.86                     | 0.40              |
| 1:1A:2033:A:O2'   | 1:1A:2034:G:O5'   | 2.21                     | 0.40              |
| 1:1A:2273:G:H2'   | 1:1A:2274:C:C6    | 2.55                     | 0.40              |
| 1:1A:2496:G:H2'   | 1:1A:2497:C:H6    | 1.81                     | 0.40              |
| 1:1A:2675:G:O2'   | 1:1A:2676:A:H8    | 2.04                     | 0.40              |
| 1:1A:2682:G:H2'   | 1:1A:2683:C:C6    | 2.56                     | 0.40              |
| 1:1A:2789:A:H1'   | 1:1A:2796:G:C1'   | 2.51                     | 0.40              |
| 1:1A:3773:U:H3'   | 1:1A:3773:U:OP2   | 2.20                     | 0.40              |
| 1:1A:4103:C:H1'   | 1:1A:4106:G:H22   | 1.85                     | 0.40              |
| 1:1A:4109:G:C2'   | 1:1A:4110:C:O4'   | 2.70                     | 0.40              |
| 1:1A:4474:A:OP2   | 1:1A:4476:C:N4    | 2.51                     | 0.40              |
| 1:1A:4689:U:H2'   | 1:1A:4690:G:O4'   | 2.21                     | 0.40              |
| 1:1A:4748:U:H2'   | 1:1A:4749:C:O4'   | 2.21                     | 0.40              |
| 1:1A:5029:C:O2'   | 1:1A:5030:U:O5'   | 2.36                     | 0.40              |
| 2:1B:19:C:H2'     | 2:1B:20:U:C6      | 2.56                     | 0.40              |
| 5:1E:98:GLY:HA2   | 17:2I:149:TYR:CE1 | 2.57                     | 0.40              |
| 5:1E:238:LYS:HB2  | 5:1E:238:LYS:HE2  | 1.89                     | 0.40              |
| 7:1G:143:THR:HA   | 7:1G:172:SER:O    | 2.22                     | 0.40              |
| 8:1H:179:LEU:HD12 | 8:1H:183:ARG:C    | 2.46                     | 0.40              |
| 8:1H:190:HIS:ND1  | 8:1H:192:LYS:HB2  | 2.37                     | 0.40              |
| 8:1H:233:PHE:HE2  | 8:1H:235:THR:CG2  | 2.34                     | 0.40              |
| 9:2A:237:GLU:HB3  | 9:2A:238:ASP:H    | 1.63                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:2B:159:HIS:CE1  | 10:2B:185:LYS:HG3  | 2.55                     | 0.40              |
| 14:2F:97:SER:O     | 14:2F:97:SER:OG    | 2.26                     | 0.40              |
| 15:2G:25:VAL:HG13  | 15:2G:26:ALA:N     | 2.36                     | 0.40              |
| 16:2H:120:TRP:CZ2  | 16:2H:122:GLY:HA2  | 2.57                     | 0.40              |
| 18:2J:10:ASN:OD1   | 18:2J:10:ASN:N     | 2.51                     | 0.40              |
| 19:2K:161:SER:O    | 19:2K:161:SER:OG   | 2.39                     | 0.40              |
| 28:2T:13:VAL:HG12  | 28:2T:19:SER:HA    | 2.02                     | 0.40              |
| 46:2L:41:TYR:HB3   | 46:2L:163:LEU:CD2  | 2.50                     | 0.40              |
| 46:2L:85:MET:HE1   | 46:2L:90:LEU:HB2   | 2.03                     | 0.40              |
| 46:2L:208:SER:OG   | 46:2L:209:THR:N    | 2.53                     | 0.40              |
| 47:2m:29:G:H2'     | 47:2m:30:C:H6      | 1.85                     | 0.40              |
| 47:2m:64:A:OP1     | 70:3H:136:LYS:NZ   | 2.31                     | 0.40              |
| 47:2m:211:G:H2'    | 47:2m:212:C:C6     | 2.56                     | 0.40              |
| 47:2m:846:G:H5''   | 47:2m:847:A:O5'    | 2.21                     | 0.40              |
| 47:2m:922:A:H2'    | 47:2m:923:G:O4'    | 2.21                     | 0.40              |
| 47:2m:1059:G:N2    | 47:2m:1829:G:H4'   | 2.36                     | 0.40              |
| 47:2m:1192:U:H2'   | 47:2m:1193:U:C6    | 2.57                     | 0.40              |
| 47:2m:1700:C:O2    | 47:2m:1834:A:N6    | 2.54                     | 0.40              |
| 49:2o:87:ILE:HG12  | 49:2o:88:THR:N     | 2.37                     | 0.40              |
| 49:2o:150:ILE:HD12 | 49:2o:151:ARG:N    | 2.36                     | 0.40              |
| 51:2q:174:LYS:HE2  | 51:2q:174:LYS:HB3  | 1.91                     | 0.40              |
| 52:2r:102:LEU:HD11 | 77:3O:108:ILE:HG23 | 2.02                     | 0.40              |
| 54:2t:143:LYS:HB2  | 54:2t:147:LYS:NZ   | 2.36                     | 0.40              |
| 56:2v:96:ILE:HD11  | 56:2v:103:GLU:OE2  | 2.21                     | 0.40              |
| 57:2w:84:ILE:HG23  | 57:2w:86:LEU:HD21  | 2.03                     | 0.40              |
| 63:3A:11:LEU:CD1   | 69:3G:79:GLU:HB3   | 2.51                     | 0.40              |
| 66:3D:31:ARG:CB    | 66:3D:43:ILE:HD13  | 2.48                     | 0.40              |
| 68:3F:139:LYS:CG   | 68:3F:140:TYR:N    | 2.83                     | 0.40              |
| 69:3G:146:GLU:OE1  | 69:3G:146:GLU:HA   | 2.21                     | 0.40              |
| 76:3N:55:ILE:N     | 76:3N:55:ILE:CD1   | 2.83                     | 0.40              |
| 76:3N:106:GLN:HG3  | 76:3N:106:GLN:H    | 1.68                     | 0.40              |
| 76:3N:111:LYS:HA   | 76:3N:114:MET:HG3  | 2.02                     | 0.40              |
| 77:3O:79:ILE:HG21  | 77:3O:84:ALA:CB    | 2.31                     | 0.40              |
| 78:3P:37:CYS:SG    | 78:3P:38:PRO:HD2   | 2.61                     | 0.40              |
| 80:3R:124:ASP:OD1  | 80:3R:125:GLU:N    | 2.53                     | 0.40              |
| 1:1A:139:G:C2'     | 1:1A:140:G:C8      | 3.04                     | 0.40              |
| 1:1A:181:C:H2'     | 1:1A:182:G:H8      | 1.86                     | 0.40              |
| 1:1A:227:A:H2'     | 1:1A:228:C:O4'     | 2.21                     | 0.40              |
| 1:1A:256:G:O2'     | 1:1A:257:C:H5'     | 2.21                     | 0.40              |
| 1:1A:434:A:H2'     | 1:1A:435:A:O4'     | 2.21                     | 0.40              |
| 1:1A:732:A:H2'     | 1:1A:733:A:O4'     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1512:G:O2'   | 1:1A:1513:U:H5'    | 2.21                     | 0.40              |
| 1:1A:1700:G:O5'   | 6:1F:306:ARG:HD3   | 2.21                     | 0.40              |
| 1:1A:2507:A:OP2   | 1:1A:2508:U:H5     | 2.05                     | 0.40              |
| 1:1A:2610:G:H2'   | 1:1A:2611:A:H8     | 1.85                     | 0.40              |
| 1:1A:2864:A:H2'   | 1:1A:2865:U:C6     | 2.56                     | 0.40              |
| 1:1A:4054:C:H4'   | 46:2l:1:MET:O      | 2.21                     | 0.40              |
| 1:1A:4209:G:O2'   | 1:1A:4210:U:H5'    | 2.21                     | 0.40              |
| 1:1A:4439:U:C2    | 1:1A:4440:G:C8     | 3.09                     | 0.40              |
| 1:1A:4568:A:N3    | 18:2J:69:ARG:NH1   | 2.66                     | 0.40              |
| 1:1A:4625:C:OP1   | 5:1E:224:LYS:HG3   | 2.21                     | 0.40              |
| 1:1A:4963:G:C2    | 1:1A:4964:C:C5     | 3.10                     | 0.40              |
| 81:1A:5115:84D:N1 | 2:1B:88:A:OP1      | 2.53                     | 0.40              |
| 2:1B:107:G:C2     | 2:1B:108:G:C8      | 3.10                     | 0.40              |
| 4:1D:107:MET:O    | 4:1D:139:HIS:NE2   | 2.52                     | 0.40              |
| 5:1E:298:LEU:C    | 5:1E:298:LEU:HD12  | 2.47                     | 0.40              |
| 13:2E:20:LEU:HB2  | 13:2E:79:ALA:HB1   | 2.03                     | 0.40              |
| 26:2R:109:ILE:O   | 26:2R:113:VAL:HG23 | 2.22                     | 0.40              |
| 27:2S:89:LYS:HD3  | 27:2S:91:ASN:HD21  | 1.86                     | 0.40              |
| 28:2T:30:ASP:HA   | 28:2T:39:SER:HB2   | 2.02                     | 0.40              |
| 39:2e:10:ASP:C    | 39:2e:10:ASP:OD1   | 2.64                     | 0.40              |
| 46:2l:60:ARG:CB   | 46:2l:61:PRO:CD    | 2.98                     | 0.40              |
| 46:2l:67:VAL:O    | 46:2l:67:VAL:HG22  | 2.21                     | 0.40              |
| 47:2m:11:A:O2'    | 47:2m:12:U:H5'     | 2.21                     | 0.40              |
| 47:2m:42:A:O2'    | 47:2m:43:U:H5'     | 2.22                     | 0.40              |
| 47:2m:373:G:OP1   | 56:2v:135:SER:OG   | 2.40                     | 0.40              |
| 47:2m:394:G:C2    | 47:2m:395:G:C8     | 3.10                     | 0.40              |
| 47:2m:459:C:H2'   | 47:2m:460:A:O4'    | 2.22                     | 0.40              |
| 47:2m:596:U:H1'   | 47:2m:645:C:O2'    | 2.21                     | 0.40              |
| 47:2m:889:U:O5'   | 47:2m:890:U:H5'    | 2.21                     | 0.40              |
| 47:2m:957:A:O2'   | 47:2m:958:G:P      | 2.79                     | 0.40              |
| 47:2m:959:G:O2'   | 47:2m:1065:G:H4'   | 2.21                     | 0.40              |
| 47:2m:1291:A:C3'  | 47:2m:1292:C:H5'   | 2.49                     | 0.40              |
| 47:2m:1301:A:H2'  | 47:2m:1303:C:C5    | 2.54                     | 0.40              |
| 47:2m:1414:A:C2   | 47:2m:1417:C:H5'   | 2.56                     | 0.40              |
| 47:2m:1434:C:H2'  | 47:2m:1435:C:C6    | 2.56                     | 0.40              |
| 47:2m:1541:G:H2'  | 47:2m:1542:C:C6    | 2.56                     | 0.40              |
| 47:2m:1607:A:H61  | 47:2m:1632:G:C2'   | 2.35                     | 0.40              |
| 47:2m:1612:G:H5'  | 60:2z:87:GLN:O     | 2.21                     | 0.40              |
| 47:2m:1658:G:H2'  | 47:2m:1659:U:O4'   | 2.22                     | 0.40              |
| 48:2n:76:VAL:C    | 48:2n:77:ILE:HD13  | 2.46                     | 0.40              |
| 49:2o:35:ALA:N    | 49:2o:42:ARG:O     | 2.35                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:2q:10:LYS:HD3   | 51:2q:10:LYS:HA    | 1.89                     | 0.40              |
| 51:2q:47:PHE:CE2   | 51:2q:90:ILE:HD12  | 2.57                     | 0.40              |
| 52:2r:175:ASP:HA   | 52:2r:178:ILE:HG12 | 2.04                     | 0.40              |
| 56:2v:124:ASP:OD2  | 56:2v:145:VAL:HG13 | 2.21                     | 0.40              |
| 57:2w:116:LEU:HD12 | 57:2w:117:GLY:N    | 2.36                     | 0.40              |
| 58:2x:8:GLN:HA     | 58:2x:99:TYR:CE1   | 2.56                     | 0.40              |
| 58:2x:39:LEU:CB    | 58:2x:51:LEU:HD21  | 2.50                     | 0.40              |
| 58:2x:54:PRO:CD    | 58:2x:88:ILE:HD11  | 2.50                     | 0.40              |
| 59:2y:125:GLY:O    | 59:2y:126:MET:HG3  | 2.21                     | 0.40              |
| 61:20:13:GLU:O     | 61:20:16:ARG:HG2   | 2.21                     | 0.40              |
| 68:3F:155:ARG:HD3  | 68:3F:155:ARG:HA   | 1.76                     | 0.40              |
| 70:3H:209:TYR:CD1  | 70:3H:209:TYR:C    | 2.99                     | 0.40              |
| 73:3K:28:LEU:HD23  | 73:3K:28:LEU:HA    | 1.84                     | 0.40              |
| 73:3K:52:VAL:HG22  | 73:3K:55:ARG:NH2   | 2.36                     | 0.40              |
| 73:3K:99:ARG:NH2   | 73:3K:115:LEU:HD21 | 2.35                     | 0.40              |
| 74:3L:12:GLU:HB3   | 74:3L:13:GLN:H     | 1.76                     | 0.40              |
| 77:3O:50:PHE:HB2   | 77:3O:54:THR:CB    | 2.50                     | 0.40              |
| 77:3O:94:LYS:HB2   | 77:3O:96:LEU:HD23  | 2.03                     | 0.40              |
| 1:1A:265:C:H1'     | 36:2b:112:ARG:NH2  | 2.34                     | 0.40              |
| 1:1A:726:G:H2'     | 1:1A:727:C:H6      | 1.86                     | 0.40              |
| 1:1A:748:G:OP1     | 21:2M:134:ALA:HB3  | 2.21                     | 0.40              |
| 1:1A:914:U:C2'     | 1:1A:915:A:OP2     | 2.69                     | 0.40              |
| 1:1A:941:C:O2'     | 1:1A:942:G:H5'     | 2.21                     | 0.40              |
| 1:1A:1241:C:O2     | 1:1A:1241:C:C3'    | 2.70                     | 0.40              |
| 1:1A:1270:A:H1'    | 1:1A:1440:U:O4'    | 2.22                     | 0.40              |
| 1:1A:1467:C:H2'    | 1:1A:1468:C:H6     | 1.86                     | 0.40              |
| 1:1A:1995:G:H2'    | 1:1A:1996:C:C6     | 2.57                     | 0.40              |
| 1:1A:2391:G:H2'    | 1:1A:2392:C:C6     | 2.56                     | 0.40              |
| 1:1A:2538:U:H2'    | 1:1A:2539:C:C6     | 2.57                     | 0.40              |
| 1:1A:2895:A:H2'    | 1:1A:2896:G:C8     | 2.56                     | 0.40              |
| 1:1A:3877:A:O2'    | 1:1A:4400:G:N2     | 2.43                     | 0.40              |
| 1:1A:4194:U:H1'    | 1:1A:4221:C:N4     | 2.37                     | 0.40              |
| 1:1A:4897:G:OP2    | 15:2G:128:LYS:NZ   | 2.54                     | 0.40              |
| 1:1A:5042:A:H2'    | 1:1A:5043:A:H8     | 1.87                     | 0.40              |
| 3:1C:155:C:C2'     | 3:1C:156:U:H5'     | 2.51                     | 0.40              |
| 7:1G:103:LEU:HG    | 7:1G:247:ILE:CG2   | 2.45                     | 0.40              |
| 7:1G:242:LYS:HB2   | 7:1G:242:LYS:NZ    | 2.37                     | 0.40              |
| 8:1H:51:VAL:HG22   | 8:1H:54:ILE:HB     | 2.03                     | 0.40              |
| 22:2N:107:LYS:NZ   | 22:2N:108:ARG:HA   | 2.35                     | 0.40              |
| 35:2a:107:LEU:O    | 35:2a:110:GLN:NE2  | 2.54                     | 0.40              |
| 46:2l:62:LYS:HD3   | 46:2l:153:SER:HB3  | 2.03                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:2m:85:A:C4'    | 47:2m:150:A:H4'    | 2.52                     | 0.40              |
| 47:2m:116:U:H2'   | 47:2m:117:C:O4'    | 2.21                     | 0.40              |
| 47:2m:141:A:C4'   | 47:2m:142:C:H5''   | 2.39                     | 0.40              |
| 47:2m:806:U:H3    | 47:2m:857:U:H3     | 1.69                     | 0.40              |
| 47:2m:903:A:C2'   | 47:2m:904:A:H5''   | 2.51                     | 0.40              |
| 47:2m:1151:G:O2'  | 47:2m:1152:U:H5'   | 2.21                     | 0.40              |
| 47:2m:1205:C:H5'  | 47:2m:1700:C:OP2   | 2.21                     | 0.40              |
| 47:2m:1256:G:H22  | 62:21:64:THR:HG23  | 1.85                     | 0.40              |
| 47:2m:1609:C:OP2  | 60:2z:132:ARG:HB2  | 2.21                     | 0.40              |
| 47:2m:1666:C:H2'  | 47:2m:1667:U:C6    | 2.57                     | 0.40              |
| 48:2n:16:LEU:HD23 | 48:2n:16:LEU:HA    | 1.85                     | 0.40              |
| 48:2n:147:LEU:HG  | 48:2n:163:CYS:SG   | 2.61                     | 0.40              |
| 49:2o:97:LEU:HB3  | 49:2o:232:HIS:CD2  | 2.57                     | 0.40              |
| 49:2o:228:LEU:HA  | 49:2o:231:LEU:HD12 | 2.02                     | 0.40              |
| 50:2p:223:ILE:CG2 | 68:3F:189:ILE:HG13 | 2.50                     | 0.40              |
| 51:2q:181:CYS:HB2 | 51:2q:226:PHE:O    | 2.22                     | 0.40              |
| 52:2r:82:ASN:HB3  | 52:2r:85:LYS:HD2   | 1.98                     | 0.40              |
| 55:2u:64:TRP:CD1  | 67:3E:23:VAL:HG13  | 2.56                     | 0.40              |
| 61:20:110:LEU:O   | 61:20:111:LYS:HB2  | 2.21                     | 0.40              |
| 65:3C:22:ARG:HA   | 65:3C:22:ARG:HD2   | 1.84                     | 0.40              |
| 68:3F:78:ALA:C    | 68:3F:89:LEU:HD12  | 2.46                     | 0.40              |
| 71:3I:22:LYS:HD2  | 71:3I:22:LYS:HA    | 1.97                     | 0.40              |
| 71:3I:60:LEU:HB2  | 71:3I:94:LEU:HD21  | 2.03                     | 0.40              |
| 73:3K:28:LEU:HD22 | 73:3K:32:ASP:OD1   | 2.20                     | 0.40              |
| 74:3L:58:GLY:O    | 74:3L:62:VAL:HG22  | 2.22                     | 0.40              |
| 74:3L:110:PRO:C   | 74:3L:113:GLN:HE21 | 2.26                     | 0.40              |
| 75:3M:43:LYS:HE2  | 75:3M:43:LYS:HB3   | 1.83                     | 0.40              |
| 1:1A:100:C:O2     | 1:1A:100:C:O4'     | 2.38                     | 0.40              |
| 1:1A:120:A:C2     | 1:1A:152:U:C2      | 3.09                     | 0.40              |
| 1:1A:952:G:H2'    | 1:1A:953:C:C6      | 2.56                     | 0.40              |
| 1:1A:1428:U:H5''  | 19:2K:42:THR:OG1   | 2.22                     | 0.40              |
| 1:1A:1580:C:H2'   | 1:1A:1581:G:O4'    | 2.21                     | 0.40              |
| 1:1A:2285:A:O2'   | 1:1A:2286:G:H5'    | 2.21                     | 0.40              |
| 1:1A:2767:U:H5''  | 1:1A:2769:U:C4     | 2.57                     | 0.40              |
| 1:1A:3974:G:H8    | 1:1A:3975:C:O4'    | 2.04                     | 0.40              |
| 1:1A:4200:G:C4    | 1:1A:4201:G:C8     | 3.09                     | 0.40              |
| 1:1A:4244:A:H2'   | 1:1A:4245:G:O4'    | 2.22                     | 0.40              |
| 1:1A:4433:G:H2'   | 1:1A:4434:C:C6     | 2.57                     | 0.40              |
| 4:1D:42:LYS:HB2   | 4:1D:89:TYR:CE2    | 2.57                     | 0.40              |
| 4:1D:147:ARG:HG3  | 4:1D:157:VAL:HG22  | 2.04                     | 0.40              |
| 5:1E:211:PHE:CE1  | 5:1E:349:LYS:HD3   | 2.57                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:53:VAL:HG11   | 7:1G:159:VAL:HA    | 2.04                     | 0.40              |
| 7:1G:228:LYS:C     | 7:1G:230:SER:H     | 2.28                     | 0.40              |
| 8:1H:165:LEU:CD2   | 8:1H:176:THR:HG22  | 2.51                     | 0.40              |
| 8:1H:209:PRO:O     | 8:1H:212:LEU:HG    | 2.21                     | 0.40              |
| 8:1H:224:LYS:N     | 8:1H:225:PRO:HD3   | 2.36                     | 0.40              |
| 9:2A:225:THR:OG1   | 9:2A:231:GLY:HA3   | 2.22                     | 0.40              |
| 10:2B:187:LYS:HE2  | 10:2B:187:LYS:HB3  | 1.86                     | 0.40              |
| 12:2D:131:ILE:HD13 | 12:2D:131:ILE:HA   | 1.90                     | 0.40              |
| 13:2E:44:THR:O     | 13:2E:78:LYS:HE3   | 2.21                     | 0.40              |
| 14:2F:50:PRO:O     | 14:2F:51:ALA:HB3   | 2.20                     | 0.40              |
| 17:2I:168:TYR:CE2  | 17:2I:172:LYS:HD3  | 2.56                     | 0.40              |
| 27:2S:108:ARG:HH11 | 27:2S:108:ARG:HG3  | 1.86                     | 0.40              |
| 46:2l:56:LYS:O     | 46:2l:182:ASN:ND2  | 2.54                     | 0.40              |
| 47:2m:35:C:H2'     | 47:2m:36:U:C6      | 2.57                     | 0.40              |
| 47:2m:610:G:C2     | 47:2m:611:G:C8     | 3.10                     | 0.40              |
| 47:2m:612:U:H2'    | 47:2m:613:G:C5'    | 2.49                     | 0.40              |
| 47:2m:651:U:H2'    | 47:2m:652:U:C6     | 2.56                     | 0.40              |
| 47:2m:812:A:O2'    | 51:2q:12:VAL:O     | 2.29                     | 0.40              |
| 47:2m:1109:C:O2'   | 47:2m:1110:G:O5'   | 2.39                     | 0.40              |
| 47:2m:1166:G:C2'   | 47:2m:1167:G:H5'   | 2.51                     | 0.40              |
| 47:2m:1312:G:H4'   | 47:2m:1314:U:O4    | 2.21                     | 0.40              |
| 47:2m:1523:C:H2'   | 47:2m:1524:G:C8    | 2.56                     | 0.40              |
| 47:2m:1546:G:OP1   | 58:2x:74:GLY:HA3   | 2.20                     | 0.40              |
| 47:2m:1610:G:C2'   | 47:2m:1611:G:O4'   | 2.69                     | 0.40              |
| 47:2m:1688:C:C2    | 47:2m:1689:C:C5    | 3.09                     | 0.40              |
| 47:2m:1714:U:H2'   | 47:2m:1715:A:H8    | 1.87                     | 0.40              |
| 50:2p:9:ARG:HA     | 50:2p:12:VAL:CG2   | 2.51                     | 0.40              |
| 53:2s:58:LYS:HB3   | 53:2s:90:LYS:HD2   | 2.03                     | 0.40              |
| 56:2v:21:LYS:O     | 56:2v:22:ARG:C     | 2.65                     | 0.40              |
| 56:2v:150:GLY:C    | 56:2v:151:THR:HG23 | 2.47                     | 0.40              |
| 59:2y:60:ARG:HD2   | 59:2y:63:ARG:HH21  | 1.86                     | 0.40              |
| 59:2y:88:VAL:O     | 59:2y:88:VAL:HG23  | 2.20                     | 0.40              |
| 63:3A:12:TYR:HB3   | 69:3G:79:GLU:HG3   | 2.03                     | 0.40              |
| 64:3B:11:ARG:HA    | 64:3B:14:ARG:CG    | 2.52                     | 0.40              |
| 68:3F:82:SER:OG    | 68:3F:83:TRP:N     | 2.54                     | 0.40              |
| 68:3F:243:PRO:HG3  | 68:3F:293:ALA:C    | 2.47                     | 0.40              |
| 70:3H:52:ILE:HG12  | 70:3H:111:LEU:HD21 | 2.03                     | 0.40              |
| 71:3I:122:SER:O    | 71:3I:123:ILE:C    | 2.64                     | 0.40              |
| 72:3J:32:ALA:HB1   | 72:3J:37:GLU:HG3   | 2.03                     | 0.40              |
| 72:3J:63:LYS:HA    | 72:3J:63:LYS:HE2   | 2.04                     | 0.40              |
| 73:3K:4:MET:SD     | 73:3K:121:ARG:HG2  | 2.61                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:3L:103:ASN:HD21 | 74:3L:140:THR:HG22 | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | 1D    | 246/257 (96%) | 227 (92%) | 19 (8%)  | 0        | 100         | 100 |
| 5   | 1E    | 400/403 (99%) | 387 (97%) | 13 (3%)  | 0        | 100         | 100 |
| 6   | 1F    | 366/427 (86%) | 344 (94%) | 22 (6%)  | 0        | 100         | 100 |
| 7   | 1G    | 291/297 (98%) | 277 (95%) | 14 (5%)  | 0        | 100         | 100 |
| 8   | 1H    | 232/288 (81%) | 210 (90%) | 22 (10%) | 0        | 100         | 100 |
| 9   | 2A    | 224/248 (90%) | 212 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 10  | 2B    | 240/266 (90%) | 227 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 11  | 2C    | 188/192 (98%) | 176 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 12  | 2D    | 211/214 (99%) | 198 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 13  | 2E    | 174/178 (98%) | 166 (95%) | 7 (4%)   | 1 (1%)   | 21          | 42  |
| 14  | 2F    | 208/211 (99%) | 192 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 15  | 2G    | 137/215 (64%) | 129 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 16  | 2H    | 201/204 (98%) | 193 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 17  | 2I    | 199/203 (98%) | 193 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 18  | 2J    | 151/184 (82%) | 144 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 19  | 2K    | 185/188 (98%) | 179 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 20  | 2L    | 185/196 (94%) | 179 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 21  | 2M    | 173/176 (98%) | 159 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 22  | 2N    | 157/160 (98%) | 153 (98%) | 4 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 23  | 2O    | 99/128 (77%)  | 85 (86%)  | 14 (14%) | 0        | 100         | 100 |
| 24  | 2P    | 129/140 (92%) | 124 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 25  | 2Q    | 122/157 (78%) | 109 (89%) | 13 (11%) | 0        | 100         | 100 |
| 26  | 2R    | 118/156 (76%) | 113 (96%) | 4 (3%)   | 1 (1%)   | 16          | 34  |
| 27  | 2S    | 132/145 (91%) | 127 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 28  | 2T    | 133/136 (98%) | 125 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 29  | 2U    | 145/148 (98%) | 141 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 30  | 2V    | 105/159 (66%) | 100 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 31  | 2W    | 96/115 (84%)  | 91 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 32  | 2X    | 105/125 (84%) | 100 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 33  | 2Y    | 126/135 (93%) | 119 (94%) | 6 (5%)   | 1 (1%)   | 16          | 34  |
| 34  | 2Z    | 107/110 (97%) | 103 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 35  | 2a    | 112/117 (96%) | 111 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 36  | 2b    | 120/123 (98%) | 117 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 37  | 2c    | 100/105 (95%) | 98 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 38  | 2d    | 85/97 (88%)   | 82 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 39  | 2e    | 67/70 (96%)   | 64 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 40  | 2f    | 48/51 (94%)   | 47 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 41  | 2g    | 49/128 (38%)  | 48 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 42  | 2h    | 22/25 (88%)   | 22 (100%) | 0        | 0        | 100         | 100 |
| 43  | 2i    | 104/106 (98%) | 100 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 44  | 2j    | 89/92 (97%)   | 85 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 45  | 2k    | 123/137 (90%) | 116 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 46  | 2l    | 215/217 (99%) | 173 (80%) | 42 (20%) | 0        | 100         | 100 |
| 48  | 2n    | 219/295 (74%) | 199 (91%) | 19 (9%)  | 1 (0%)   | 24          | 46  |
| 49  | 2o    | 212/264 (80%) | 204 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 50  | 2p    | 225/243 (93%) | 204 (91%) | 21 (9%)  | 0        | 100         | 100 |
| 51  | 2q    | 260/263 (99%) | 247 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 52  | 2r    | 187/204 (92%) | 169 (90%) | 18 (10%) | 0        | 100         | 100 |
| 53  | 2s    | 182/194 (94%) | 159 (87%) | 22 (12%) | 1 (0%)   | 24          | 46  |
| 54  | 2t    | 204/208 (98%) | 193 (95%) | 11 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 55  | 2u    | 96/165 (58%)      | 85 (88%)    | 11 (12%) | 0        | 100         | 100 |
| 56  | 2v    | 151/158 (96%)     | 138 (91%)   | 12 (8%)  | 1 (1%)   | 18          | 38  |
| 57  | 2w    | 125/145 (86%)     | 116 (93%)   | 9 (7%)   | 0        | 100         | 100 |
| 58  | 2x    | 139/146 (95%)     | 127 (91%)   | 12 (9%)  | 0        | 100         | 100 |
| 59  | 2y    | 133/135 (98%)     | 118 (89%)   | 15 (11%) | 0        | 100         | 100 |
| 60  | 2z    | 143/152 (94%)     | 131 (92%)   | 12 (8%)  | 0        | 100         | 100 |
| 61  | 20    | 141/145 (97%)     | 129 (92%)   | 12 (8%)  | 0        | 100         | 100 |
| 62  | 21    | 101/119 (85%)     | 95 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| 63  | 3A    | 81/83 (98%)       | 72 (89%)    | 9 (11%)  | 0        | 100         | 100 |
| 64  | 3B    | 139/143 (97%)     | 130 (94%)   | 9 (6%)   | 0        | 100         | 100 |
| 65  | 3C    | 101/115 (88%)     | 95 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| 66  | 3D    | 62/69 (90%)       | 51 (82%)    | 11 (18%) | 0        | 100         | 100 |
| 67  | 3E    | 53/56 (95%)       | 51 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 68  | 3F    | 311/317 (98%)     | 283 (91%)   | 28 (9%)  | 0        | 100         | 100 |
| 69  | 3G    | 221/293 (75%)     | 204 (92%)   | 17 (8%)  | 0        | 100         | 100 |
| 70  | 3H    | 235/249 (94%)     | 228 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 71  | 3I    | 184/194 (95%)     | 167 (91%)   | 17 (9%)  | 0        | 100         | 100 |
| 72  | 3J    | 120/132 (91%)     | 113 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 73  | 3K    | 148/151 (98%)     | 145 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 74  | 3L    | 138/151 (91%)     | 125 (91%)   | 13 (9%)  | 0        | 100         | 100 |
| 75  | 3M    | 127/130 (98%)     | 122 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 76  | 3N    | 130/133 (98%)     | 127 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 77  | 3O    | 73/125 (58%)      | 61 (84%)    | 12 (16%) | 0        | 100         | 100 |
| 78  | 3P    | 81/84 (96%)       | 73 (90%)    | 8 (10%)  | 0        | 100         | 100 |
| 79  | 3Q    | 56/59 (95%)       | 51 (91%)    | 5 (9%)   | 0        | 100         | 100 |
| 80  | 3R    | 65/156 (42%)      | 61 (94%)    | 4 (6%)   | 0        | 100         | 100 |
| All | All   | 11562/12905 (90%) | 10818 (94%) | 738 (6%) | 6 (0%)   | 49          | 70  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | 2R    | 38  | LYS  |
| 33  | 2Y    | 92  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 2s    | 15  | LYS  |
| 48  | 2n    | 28  | THR  |
| 13  | 2E    | 175 | LEU  |
| 56  | 2v    | 151 | THR  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | 1D    | 190/199 (96%)  | 184 (97%) | 6 (3%)   | 34          | 62 |
| 5   | 1E    | 348/349 (100%) | 336 (97%) | 12 (3%)  | 32          | 60 |
| 6   | 1F    | 306/348 (88%)  | 296 (97%) | 10 (3%)  | 33          | 61 |
| 7   | 1G    | 246/250 (98%)  | 235 (96%) | 11 (4%)  | 24          | 50 |
| 8   | 1H    | 209/252 (83%)  | 193 (92%) | 16 (8%)  | 12          | 27 |
| 9   | 2A    | 195/215 (91%)  | 191 (98%) | 4 (2%)   | 47          | 73 |
| 10  | 2B    | 204/223 (92%)  | 195 (96%) | 9 (4%)   | 25          | 50 |
| 11  | 2C    | 169/171 (99%)  | 159 (94%) | 10 (6%)  | 18          | 38 |
| 12  | 2D    | 180/181 (99%)  | 174 (97%) | 6 (3%)   | 33          | 61 |
| 13  | 2E    | 148/149 (99%)  | 141 (95%) | 7 (5%)   | 23          | 48 |
| 14  | 2F    | 176/177 (99%)  | 166 (94%) | 10 (6%)  | 18          | 40 |
| 15  | 2G    | 118/161 (73%)  | 112 (95%) | 6 (5%)   | 21          | 45 |
| 16  | 2H    | 171/172 (99%)  | 165 (96%) | 6 (4%)   | 32          | 59 |
| 17  | 2I    | 173/174 (99%)  | 169 (98%) | 4 (2%)   | 44          | 71 |
| 18  | 2J    | 134/163 (82%)  | 128 (96%) | 6 (4%)   | 24          | 50 |
| 19  | 2K    | 164/165 (99%)  | 160 (98%) | 4 (2%)   | 43          | 70 |
| 20  | 2L    | 166/175 (95%)  | 160 (96%) | 6 (4%)   | 31          | 58 |
| 21  | 2M    | 156/157 (99%)  | 148 (95%) | 8 (5%)   | 21          | 45 |
| 22  | 2N    | 139/140 (99%)  | 131 (94%) | 8 (6%)   | 18          | 39 |
| 23  | 2O    | 91/115 (79%)   | 82 (90%)  | 9 (10%)  | 7           | 16 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 24  | 2P    | 101/107 (94%)  | 96 (95%)   | 5 (5%)   | 22          | 46  |
| 25  | 2Q    | 103/126 (82%)  | 103 (100%) | 0        | 100         | 100 |
| 26  | 2R    | 108/133 (81%)  | 104 (96%)  | 4 (4%)   | 30          | 57  |
| 27  | 2S    | 124/135 (92%)  | 122 (98%)  | 2 (2%)   | 55          | 79  |
| 28  | 2T    | 117/118 (99%)  | 110 (94%)  | 7 (6%)   | 17          | 37  |
| 29  | 2U    | 120/121 (99%)  | 114 (95%)  | 6 (5%)   | 22          | 46  |
| 30  | 2V    | 89/126 (71%)   | 84 (94%)   | 5 (6%)   | 19          | 40  |
| 31  | 2W    | 83/97 (86%)    | 78 (94%)   | 5 (6%)   | 17          | 37  |
| 32  | 2X    | 98/110 (89%)   | 90 (92%)   | 8 (8%)   | 10          | 24  |
| 33  | 2Y    | 114/121 (94%)  | 111 (97%)  | 3 (3%)   | 40          | 68  |
| 34  | 2Z    | 88/89 (99%)    | 86 (98%)   | 2 (2%)   | 44          | 71  |
| 35  | 2a    | 98/100 (98%)   | 93 (95%)   | 5 (5%)   | 21          | 45  |
| 36  | 2b    | 109/110 (99%)  | 104 (95%)  | 5 (5%)   | 24          | 49  |
| 37  | 2c    | 86/89 (97%)    | 82 (95%)   | 4 (5%)   | 23          | 48  |
| 38  | 2d    | 74/80 (92%)    | 69 (93%)   | 5 (7%)   | 14          | 32  |
| 39  | 2e    | 64/65 (98%)    | 58 (91%)   | 6 (9%)   | 8           | 18  |
| 40  | 2f    | 47/48 (98%)    | 45 (96%)   | 2 (4%)   | 26          | 51  |
| 41  | 2g    | 47/115 (41%)   | 46 (98%)   | 1 (2%)   | 47          | 73  |
| 42  | 2h    | 23/24 (96%)    | 22 (96%)   | 1 (4%)   | 26          | 51  |
| 43  | 2i    | 94/94 (100%)   | 91 (97%)   | 3 (3%)   | 34          | 62  |
| 44  | 2j    | 74/75 (99%)    | 67 (90%)   | 7 (10%)  | 8           | 18  |
| 45  | 2k    | 109/121 (90%)  | 103 (94%)  | 6 (6%)   | 19          | 41  |
| 46  | 2l    | 195/196 (100%) | 186 (95%)  | 9 (5%)   | 24          | 49  |
| 48  | 2n    | 183/243 (75%)  | 163 (89%)  | 20 (11%) | 6           | 13  |
| 49  | 2o    | 195/231 (84%)  | 181 (93%)  | 14 (7%)  | 13          | 30  |
| 50  | 2p    | 190/202 (94%)  | 173 (91%)  | 17 (9%)  | 9           | 20  |
| 51  | 2q    | 224/225 (100%) | 214 (96%)  | 10 (4%)  | 24          | 50  |
| 52  | 2r    | 159/170 (94%)  | 148 (93%)  | 11 (7%)  | 14          | 32  |
| 53  | 2s    | 166/174 (95%)  | 153 (92%)  | 13 (8%)  | 11          | 26  |
| 54  | 2t    | 178/180 (99%)  | 172 (97%)  | 6 (3%)   | 32          | 60  |
| 55  | 2u    | 89/136 (65%)   | 86 (97%)   | 3 (3%)   | 32          | 60  |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-------------------|------------|----------|-------------|----|
| 56  | 2v    | 137/142 (96%)     | 129 (94%)  | 8 (6%)   | 18          | 39 |
| 57  | 2w    | 113/130 (87%)     | 111 (98%)  | 2 (2%)   | 51          | 76 |
| 58  | 2x    | 117/121 (97%)     | 108 (92%)  | 9 (8%)   | 12          | 27 |
| 59  | 2y    | 122/122 (100%)    | 110 (90%)  | 12 (10%) | 7           | 17 |
| 60  | 2z    | 126/132 (96%)     | 119 (94%)  | 7 (6%)   | 19          | 40 |
| 61  | 20    | 113/115 (98%)     | 105 (93%)  | 8 (7%)   | 13          | 31 |
| 62  | 21    | 94/107 (88%)      | 87 (93%)   | 7 (7%)   | 13          | 29 |
| 63  | 3A    | 67/67 (100%)      | 58 (87%)   | 9 (13%)  | 4           | 7  |
| 64  | 3B    | 113/115 (98%)     | 104 (92%)  | 9 (8%)   | 11          | 25 |
| 65  | 3C    | 90/98 (92%)       | 84 (93%)   | 6 (7%)   | 15          | 33 |
| 66  | 3D    | 57/62 (92%)       | 53 (93%)   | 4 (7%)   | 14          | 31 |
| 67  | 3E    | 48/49 (98%)       | 46 (96%)   | 2 (4%)   | 26          | 52 |
| 68  | 3F    | 272/275 (99%)     | 252 (93%)  | 20 (7%)  | 13          | 29 |
| 69  | 3G    | 189/225 (84%)     | 182 (96%)  | 7 (4%)   | 30          | 57 |
| 70  | 3H    | 207/218 (95%)     | 193 (93%)  | 14 (7%)  | 14          | 32 |
| 71  | 3I    | 162/168 (96%)     | 158 (98%)  | 4 (2%)   | 42          | 69 |
| 72  | 3J    | 102/108 (94%)     | 97 (95%)   | 5 (5%)   | 22          | 47 |
| 73  | 3K    | 130/131 (99%)     | 122 (94%)  | 8 (6%)   | 16          | 36 |
| 74  | 3L    | 110/119 (92%)     | 102 (93%)  | 8 (7%)   | 13          | 29 |
| 75  | 3M    | 112/113 (99%)     | 104 (93%)  | 8 (7%)   | 13          | 31 |
| 76  | 3N    | 114/115 (99%)     | 109 (96%)  | 5 (4%)   | 25          | 50 |
| 77  | 3O    | 66/103 (64%)      | 57 (86%)   | 9 (14%)  | 3           | 7  |
| 78  | 3P    | 75/76 (99%)       | 69 (92%)   | 6 (8%)   | 11          | 25 |
| 79  | 3Q    | 47/48 (98%)       | 43 (92%)   | 4 (8%)   | 10          | 22 |
| 80  | 3R    | 60/140 (43%)      | 57 (95%)   | 3 (5%)   | 22          | 46 |
| All | All   | 10075/10996 (92%) | 9538 (95%) | 537 (5%) | 22          | 43 |

All (537) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1D    | 4   | VAL  |
| 4   | 1D    | 15  | VAL  |
| 4   | 1D    | 102 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1D    | 106 | THR  |
| 4   | 1D    | 116 | LEU  |
| 4   | 1D    | 241 | ARG  |
| 5   | 1E    | 38  | SER  |
| 5   | 1E    | 135 | LYS  |
| 5   | 1E    | 194 | LEU  |
| 5   | 1E    | 215 | GLU  |
| 5   | 1E    | 257 | TRP  |
| 5   | 1E    | 258 | HIS  |
| 5   | 1E    | 289 | GLN  |
| 5   | 1E    | 292 | LEU  |
| 5   | 1E    | 299 | ILE  |
| 5   | 1E    | 304 | SER  |
| 5   | 1E    | 305 | THR  |
| 5   | 1E    | 363 | ILE  |
| 6   | 1F    | 8   | ILE  |
| 6   | 1F    | 14  | LYS  |
| 6   | 1F    | 61  | GLN  |
| 6   | 1F    | 157 | LYS  |
| 6   | 1F    | 158 | VAL  |
| 6   | 1F    | 208 | CYS  |
| 6   | 1F    | 230 | LEU  |
| 6   | 1F    | 312 | ARG  |
| 6   | 1F    | 334 | THR  |
| 6   | 1F    | 345 | ARG  |
| 7   | 1G    | 37  | VAL  |
| 7   | 1G    | 41  | LYS  |
| 7   | 1G    | 88  | VAL  |
| 7   | 1G    | 93  | THR  |
| 7   | 1G    | 154 | THR  |
| 7   | 1G    | 163 | LEU  |
| 7   | 1G    | 194 | VAL  |
| 7   | 1G    | 220 | LYS  |
| 7   | 1G    | 224 | SER  |
| 7   | 1G    | 280 | VAL  |
| 7   | 1G    | 286 | SER  |
| 8   | 1H    | 49  | VAL  |
| 8   | 1H    | 89  | LEU  |
| 8   | 1H    | 91  | THR  |
| 8   | 1H    | 96  | VAL  |
| 8   | 1H    | 106 | VAL  |
| 8   | 1H    | 128 | HIS  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 8   | 1H    | 145    | THR  |
| 8   | 1H    | 175    | VAL  |
| 8   | 1H    | 191    | GLN  |
| 8   | 1H    | 194    | VAL  |
| 8   | 1H    | 198    | SER  |
| 8   | 1H    | 221    | LYS  |
| 8   | 1H    | 235    | THR  |
| 8   | 1H    | 245    | GLN  |
| 8   | 1H    | 255    | SER  |
| 8   | 1H    | 257    | ILE  |
| 9   | 2A    | 102    | SER  |
| 9   | 2A    | 215    | SER  |
| 9   | 2A    | 247    | MET  |
| 9   | 2A    | 248    | ASN  |
| 10  | 2B    | 43     | GLN  |
| 10  | 2B    | 94     | GLN  |
| 10  | 2B    | 111    | LYS  |
| 10  | 2B    | 137[A] | ARG  |
| 10  | 2B    | 137[B] | ARG  |
| 10  | 2B    | 207    | VAL  |
| 10  | 2B    | 209    | SER  |
| 10  | 2B    | 211    | ASP  |
| 10  | 2B    | 253    | LEU  |
| 11  | 2C    | 16     | VAL  |
| 11  | 2C    | 19     | THR  |
| 11  | 2C    | 28     | LYS  |
| 11  | 2C    | 57     | VAL  |
| 11  | 2C    | 94     | SER  |
| 11  | 2C    | 140    | GLN  |
| 11  | 2C    | 155    | SER  |
| 11  | 2C    | 161    | ILE  |
| 11  | 2C    | 172    | ILE  |
| 11  | 2C    | 188    | GLN  |
| 12  | 2D    | 13     | LYS  |
| 12  | 2D    | 26     | VAL  |
| 12  | 2D    | 39     | LYS  |
| 12  | 2D    | 40     | LYS  |
| 12  | 2D    | 125    | THR  |
| 12  | 2D    | 134    | VAL  |
| 13  | 2E    | 33     | LEU  |
| 13  | 2E    | 42     | GLN  |
| 13  | 2E    | 60     | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | 2E    | 68  | ILE  |
| 13  | 2E    | 72  | CYS  |
| 13  | 2E    | 83  | LEU  |
| 13  | 2E    | 158 | SER  |
| 14  | 2F    | 42  | LYS  |
| 14  | 2F    | 52  | SER  |
| 14  | 2F    | 59  | VAL  |
| 14  | 2F    | 63  | THR  |
| 14  | 2F    | 64  | VAL  |
| 14  | 2F    | 70  | VAL  |
| 14  | 2F    | 90  | VAL  |
| 14  | 2F    | 94  | ILE  |
| 14  | 2F    | 121 | ARG  |
| 14  | 2F    | 135 | LYS  |
| 15  | 2G    | 25  | VAL  |
| 15  | 2G    | 31  | ILE  |
| 15  | 2G    | 33  | GLN  |
| 15  | 2G    | 38  | VAL  |
| 15  | 2G    | 124 | LYS  |
| 15  | 2G    | 130 | LEU  |
| 16  | 2H    | 25  | VAL  |
| 16  | 2H    | 37  | HIS  |
| 16  | 2H    | 50  | ARG  |
| 16  | 2H    | 60  | VAL  |
| 16  | 2H    | 155 | VAL  |
| 16  | 2H    | 182 | HIS  |
| 17  | 2I    | 4   | VAL  |
| 17  | 2I    | 27  | VAL  |
| 17  | 2I    | 145 | VAL  |
| 17  | 2I    | 152 | VAL  |
| 18  | 2J    | 7   | ASP  |
| 18  | 2J    | 12  | THR  |
| 18  | 2J    | 24  | VAL  |
| 18  | 2J    | 36  | ILE  |
| 18  | 2J    | 53  | LEU  |
| 18  | 2J    | 108 | ASP  |
| 19  | 2K    | 45  | GLN  |
| 19  | 2K    | 92  | VAL  |
| 19  | 2K    | 161 | SER  |
| 19  | 2K    | 167 | VAL  |
| 20  | 2L    | 20  | LYS  |
| 20  | 2L    | 57  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | 2L    | 67  | THR  |
| 20  | 2L    | 78  | ILE  |
| 20  | 2L    | 81  | ARG  |
| 20  | 2L    | 137 | ILE  |
| 21  | 2M    | 19  | THR  |
| 21  | 2M    | 48  | VAL  |
| 21  | 2M    | 90  | THR  |
| 21  | 2M    | 125 | GLN  |
| 21  | 2M    | 129 | VAL  |
| 21  | 2M    | 135 | SER  |
| 21  | 2M    | 161 | ARG  |
| 21  | 2M    | 169 | THR  |
| 22  | 2N    | 2   | THR  |
| 22  | 2N    | 4   | THR  |
| 22  | 2N    | 29  | THR  |
| 22  | 2N    | 76  | VAL  |
| 22  | 2N    | 83  | LYS  |
| 22  | 2N    | 109 | VAL  |
| 22  | 2N    | 128 | LEU  |
| 22  | 2N    | 150 | LEU  |
| 23  | 2O    | 26  | THR  |
| 23  | 2O    | 47  | ILE  |
| 23  | 2O    | 62  | THR  |
| 23  | 2O    | 76  | VAL  |
| 23  | 2O    | 79  | SER  |
| 23  | 2O    | 95  | ASN  |
| 23  | 2O    | 96  | LEU  |
| 23  | 2O    | 98  | ASP  |
| 23  | 2O    | 101 | ARG  |
| 24  | 2P    | 20  | LEU  |
| 24  | 2P    | 22  | VAL  |
| 24  | 2P    | 65  | VAL  |
| 24  | 2P    | 94  | VAL  |
| 24  | 2P    | 111 | GLU  |
| 26  | 2R    | 54  | LEU  |
| 26  | 2R    | 85  | SER  |
| 26  | 2R    | 95  | THR  |
| 26  | 2R    | 147 | LEU  |
| 27  | 2S    | 46  | SER  |
| 27  | 2S    | 105 | VAL  |
| 28  | 2T    | 24  | VAL  |
| 28  | 2T    | 60  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | 2T    | 86  | SER  |
| 28  | 2T    | 87  | VAL  |
| 28  | 2T    | 91  | LEU  |
| 28  | 2T    | 100 | VAL  |
| 28  | 2T    | 115 | LYS  |
| 29  | 2U    | 15  | VAL  |
| 29  | 2U    | 63  | LEU  |
| 29  | 2U    | 88  | VAL  |
| 29  | 2U    | 95  | THR  |
| 29  | 2U    | 103 | VAL  |
| 29  | 2U    | 140 | VAL  |
| 30  | 2V    | 4   | SER  |
| 30  | 2V    | 9   | THR  |
| 30  | 2V    | 13  | SER  |
| 30  | 2V    | 26  | SER  |
| 30  | 2V    | 93  | LEU  |
| 31  | 2W    | 24  | SER  |
| 31  | 2W    | 28  | VAL  |
| 31  | 2W    | 35  | LEU  |
| 31  | 2W    | 91  | VAL  |
| 31  | 2W    | 93  | THR  |
| 32  | 2X    | 31  | LYS  |
| 32  | 2X    | 33  | ILE  |
| 32  | 2X    | 62  | VAL  |
| 32  | 2X    | 67  | ARG  |
| 32  | 2X    | 89  | SER  |
| 32  | 2X    | 98  | SER  |
| 32  | 2X    | 100 | ASN  |
| 32  | 2X    | 101 | LYS  |
| 33  | 2Y    | 21  | ILE  |
| 33  | 2Y    | 87  | VAL  |
| 33  | 2Y    | 117 | GLN  |
| 34  | 2Z    | 33  | VAL  |
| 34  | 2Z    | 108 | SER  |
| 35  | 2a    | 23  | SER  |
| 35  | 2a    | 63  | VAL  |
| 35  | 2a    | 103 | VAL  |
| 35  | 2a    | 104 | VAL  |
| 35  | 2a    | 107 | LEU  |
| 36  | 2b    | 33  | VAL  |
| 36  | 2b    | 36  | VAL  |
| 36  | 2b    | 37  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 2b    | 46  | LYS  |
| 36  | 2b    | 71  | LYS  |
| 37  | 2c    | 29  | ARG  |
| 37  | 2c    | 81  | ILE  |
| 37  | 2c    | 93  | VAL  |
| 37  | 2c    | 94  | LEU  |
| 38  | 2d    | 6   | SER  |
| 38  | 2d    | 22  | CYS  |
| 38  | 2d    | 24  | SER  |
| 38  | 2d    | 32  | SER  |
| 38  | 2d    | 82  | THR  |
| 39  | 2e    | 8   | ILE  |
| 39  | 2e    | 18  | LYS  |
| 39  | 2e    | 22  | SER  |
| 39  | 2e    | 44  | THR  |
| 39  | 2e    | 47  | ILE  |
| 39  | 2e    | 59  | SER  |
| 40  | 2f    | 8   | ARG  |
| 40  | 2f    | 35  | ILE  |
| 41  | 2g    | 78  | ILE  |
| 42  | 2h    | 13  | LEU  |
| 43  | 2i    | 2   | VAL  |
| 43  | 2i    | 10  | THR  |
| 43  | 2i    | 104 | ILE  |
| 44  | 2j    | 26  | VAL  |
| 44  | 2j    | 29  | ILE  |
| 44  | 2j    | 36  | LYS  |
| 44  | 2j    | 72  | ASN  |
| 44  | 2j    | 79  | VAL  |
| 44  | 2j    | 81  | SER  |
| 44  | 2j    | 83  | ILE  |
| 45  | 2k    | 21  | ASN  |
| 45  | 2k    | 24  | THR  |
| 45  | 2k    | 32  | LEU  |
| 45  | 2k    | 49  | VAL  |
| 45  | 2k    | 78  | VAL  |
| 45  | 2k    | 115 | SER  |
| 46  | 2l    | 45  | LYS  |
| 46  | 2l    | 56  | LYS  |
| 46  | 2l    | 58  | THR  |
| 46  | 2l    | 73  | HIS  |
| 46  | 2l    | 78  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | 2l    | 148 | VAL  |
| 46  | 2l    | 167 | VAL  |
| 46  | 2l    | 175 | THR  |
| 46  | 2l    | 204 | LEU  |
| 48  | 2n    | 7   | VAL  |
| 48  | 2n    | 16  | LEU  |
| 48  | 2n    | 25  | LEU  |
| 48  | 2n    | 28  | THR  |
| 48  | 2n    | 38  | ILE  |
| 48  | 2n    | 51  | LEU  |
| 48  | 2n    | 54  | THR  |
| 48  | 2n    | 66  | VAL  |
| 48  | 2n    | 76  | VAL  |
| 48  | 2n    | 78  | SER  |
| 48  | 2n    | 80  | ARG  |
| 48  | 2n    | 82  | THR  |
| 48  | 2n    | 88  | LEU  |
| 48  | 2n    | 104 | THR  |
| 48  | 2n    | 118 | GLU  |
| 48  | 2n    | 125 | THR  |
| 48  | 2n    | 126 | ASP  |
| 48  | 2n    | 134 | LEU  |
| 48  | 2n    | 144 | THR  |
| 48  | 2n    | 170 | SER  |
| 49  | 2o    | 50  | THR  |
| 49  | 2o    | 55  | THR  |
| 49  | 2o    | 60  | ASP  |
| 49  | 2o    | 70  | SER  |
| 49  | 2o    | 86  | LEU  |
| 49  | 2o    | 131 | ASP  |
| 49  | 2o    | 139 | CYS  |
| 49  | 2o    | 147 | ASN  |
| 49  | 2o    | 184 | VAL  |
| 49  | 2o    | 189 | ILE  |
| 49  | 2o    | 192 | SER  |
| 49  | 2o    | 199 | LYS  |
| 49  | 2o    | 212 | VAL  |
| 49  | 2o    | 222 | LYS  |
| 50  | 2p    | 3   | VAL  |
| 50  | 2p    | 17  | PHE  |
| 50  | 2p    | 29  | LEU  |
| 50  | 2p    | 37  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | 2p    | 46  | THR  |
| 50  | 2p    | 47  | GLU  |
| 50  | 2p    | 49  | ILE  |
| 50  | 2p    | 84  | VAL  |
| 50  | 2p    | 109 | LEU  |
| 50  | 2p    | 129 | SER  |
| 50  | 2p    | 148 | LYS  |
| 50  | 2p    | 170 | THR  |
| 50  | 2p    | 181 | VAL  |
| 50  | 2p    | 198 | ILE  |
| 50  | 2p    | 206 | ASP  |
| 50  | 2p    | 209 | SER  |
| 50  | 2p    | 221 | THR  |
| 51  | 2q    | 12  | VAL  |
| 51  | 2q    | 48  | LEU  |
| 51  | 2q    | 64  | ILE  |
| 51  | 2q    | 69  | PHE  |
| 51  | 2q    | 111 | VAL  |
| 51  | 2q    | 136 | ILE  |
| 51  | 2q    | 139 | LEU  |
| 51  | 2q    | 143 | ASP  |
| 51  | 2q    | 216 | ASN  |
| 51  | 2q    | 233 | LYS  |
| 52  | 2r    | 16  | ASP  |
| 52  | 2r    | 27  | ASP  |
| 52  | 2r    | 39  | ILE  |
| 52  | 2r    | 45  | TYR  |
| 52  | 2r    | 93  | VAL  |
| 52  | 2r    | 94  | LYS  |
| 52  | 2r    | 106 | GLU  |
| 52  | 2r    | 119 | SER  |
| 52  | 2r    | 124 | ASP  |
| 52  | 2r    | 139 | VAL  |
| 52  | 2r    | 173 | LEU  |
| 53  | 2s    | 8   | ILE  |
| 53  | 2s    | 23  | ILE  |
| 53  | 2s    | 25  | GLN  |
| 53  | 2s    | 51  | ILE  |
| 53  | 2s    | 93  | VAL  |
| 53  | 2s    | 98  | ARG  |
| 53  | 2s    | 106 | ARG  |
| 53  | 2s    | 107 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | 2s    | 125 | VAL  |
| 53  | 2s    | 170 | VAL  |
| 53  | 2s    | 172 | THR  |
| 53  | 2s    | 174 | SER  |
| 53  | 2s    | 184 | ASP  |
| 54  | 2t    | 3   | ILE  |
| 54  | 2t    | 17  | LYS  |
| 54  | 2t    | 46  | VAL  |
| 54  | 2t    | 124 | LYS  |
| 54  | 2t    | 139 | LYS  |
| 54  | 2t    | 157 | LYS  |
| 55  | 2u    | 45  | VAL  |
| 55  | 2u    | 53  | LYS  |
| 55  | 2u    | 73  | ASN  |
| 56  | 2v    | 19  | ASN  |
| 56  | 2v    | 25  | LEU  |
| 56  | 2v    | 45  | LYS  |
| 56  | 2v    | 74  | SER  |
| 56  | 2v    | 91  | ASP  |
| 56  | 2v    | 125 | ILE  |
| 56  | 2v    | 126 | VAL  |
| 56  | 2v    | 135 | SER  |
| 57  | 2w    | 25  | LEU  |
| 57  | 2w    | 55  | SER  |
| 58  | 2x    | 7   | LEU  |
| 58  | 2x    | 10  | VAL  |
| 58  | 2x    | 17  | LYS  |
| 58  | 2x    | 20  | THR  |
| 58  | 2x    | 34  | VAL  |
| 58  | 2x    | 42  | ILE  |
| 58  | 2x    | 46  | THR  |
| 58  | 2x    | 114 | GLN  |
| 58  | 2x    | 121 | VAL  |
| 59  | 2y    | 6   | THR  |
| 59  | 2y    | 8   | THR  |
| 59  | 2y    | 16  | ILE  |
| 59  | 2y    | 26  | ASN  |
| 59  | 2y    | 37  | GLU  |
| 59  | 2y    | 40  | ILE  |
| 59  | 2y    | 58  | MET  |
| 59  | 2y    | 77  | GLU  |
| 59  | 2y    | 82  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | 2y    | 85  | VAL  |
| 59  | 2y    | 92  | ASP  |
| 59  | 2y    | 102 | THR  |
| 60  | 2z    | 17  | ASN  |
| 60  | 2z    | 18  | THR  |
| 60  | 2z    | 36  | VAL  |
| 60  | 2z    | 43  | VAL  |
| 60  | 2z    | 50  | ILE  |
| 60  | 2z    | 101 | ASN  |
| 60  | 2z    | 139 | THR  |
| 61  | 20    | 6   | VAL  |
| 61  | 20    | 55  | THR  |
| 61  | 20    | 60  | THR  |
| 61  | 20    | 90  | SER  |
| 61  | 20    | 96  | SER  |
| 61  | 20    | 123 | LEU  |
| 61  | 20    | 134 | ILE  |
| 61  | 20    | 138 | VAL  |
| 62  | 21    | 20  | ILE  |
| 62  | 21    | 25  | THR  |
| 62  | 21    | 59  | LYS  |
| 62  | 21    | 63  | ILE  |
| 62  | 21    | 81  | GLN  |
| 62  | 21    | 89  | ILE  |
| 62  | 21    | 114 | VAL  |
| 63  | 3A    | 22  | ARG  |
| 63  | 3A    | 33  | GLN  |
| 63  | 3A    | 39  | VAL  |
| 63  | 3A    | 43  | THR  |
| 63  | 3A    | 50  | PHE  |
| 63  | 3A    | 65  | SER  |
| 63  | 3A    | 79  | VAL  |
| 63  | 3A    | 80  | SER  |
| 63  | 3A    | 83  | PHE  |
| 64  | 3B    | 7   | LEU  |
| 64  | 3B    | 32  | LEU  |
| 64  | 3B    | 57  | VAL  |
| 64  | 3B    | 64  | SER  |
| 64  | 3B    | 70  | VAL  |
| 64  | 3B    | 72  | VAL  |
| 64  | 3B    | 100 | VAL  |
| 64  | 3B    | 122 | VAL  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 64  | 3B    | 140   | ARG  |
| 65  | 3C    | 10    | ARG  |
| 65  | 3C    | 45    | VAL  |
| 65  | 3C    | 50    | VAL  |
| 65  | 3C    | 60    | ASP  |
| 65  | 3C    | 85[A] | ARG  |
| 65  | 3C    | 85[B] | ARG  |
| 66  | 3D    | 6     | VAL  |
| 66  | 3D    | 23    | SER  |
| 66  | 3D    | 46    | VAL  |
| 66  | 3D    | 60    | GLU  |
| 67  | 3E    | 3     | HIS  |
| 67  | 3E    | 8     | TRP  |
| 68  | 3F    | 19    | THR  |
| 68  | 3F    | 23    | THR  |
| 68  | 3F    | 26    | GLN  |
| 68  | 3F    | 40    | ILE  |
| 68  | 3F    | 56    | GLN  |
| 68  | 3F    | 86    | THR  |
| 68  | 3F    | 96    | THR  |
| 68  | 3F    | 101   | PHE  |
| 68  | 3F    | 120   | ILE  |
| 68  | 3F    | 134   | THR  |
| 68  | 3F    | 141   | THR  |
| 68  | 3F    | 142   | VAL  |
| 68  | 3F    | 164   | ILE  |
| 68  | 3F    | 165   | ILE  |
| 68  | 3F    | 176   | VAL  |
| 68  | 3F    | 189   | ILE  |
| 68  | 3F    | 236   | ILE  |
| 68  | 3F    | 289   | LEU  |
| 68  | 3F    | 308   | ARG  |
| 68  | 3F    | 314   | ILE  |
| 69  | 3G    | 64    | THR  |
| 69  | 3G    | 134   | ASN  |
| 69  | 3G    | 137   | VAL  |
| 69  | 3G    | 227   | ARG  |
| 69  | 3G    | 258   | GLU  |
| 69  | 3G    | 260   | VAL  |
| 69  | 3G    | 264   | SER  |
| 70  | 3H    | 15    | LEU  |
| 70  | 3H    | 26    | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 70  | 3H    | 34     | THR  |
| 70  | 3H    | 68     | LEU  |
| 70  | 3H    | 73     | VAL  |
| 70  | 3H    | 82     | SER  |
| 70  | 3H    | 97     | VAL  |
| 70  | 3H    | 125    | THR  |
| 70  | 3H    | 128    | THR  |
| 70  | 3H    | 162    | LEU  |
| 70  | 3H    | 180    | VAL  |
| 70  | 3H    | 181    | THR  |
| 70  | 3H    | 186    | GLN  |
| 70  | 3H    | 217    | MET  |
| 71  | 3I    | 14     | VAL  |
| 71  | 3I    | 93     | LYS  |
| 71  | 3I    | 138[A] | ARG  |
| 71  | 3I    | 138[B] | ARG  |
| 72  | 3J    | 35     | ILE  |
| 72  | 3J    | 49     | LEU  |
| 72  | 3J    | 57     | ASP  |
| 72  | 3J    | 109    | VAL  |
| 72  | 3J    | 123    | VAL  |
| 73  | 3K    | 3      | ARG  |
| 73  | 3K    | 36     | GLN  |
| 73  | 3K    | 46     | THR  |
| 73  | 3K    | 80     | LEU  |
| 73  | 3K    | 87     | ASP  |
| 73  | 3K    | 99     | ARG  |
| 73  | 3K    | 143    | SER  |
| 73  | 3K    | 144    | SER  |
| 74  | 3L    | 16     | SER  |
| 74  | 3L    | 25     | GLU  |
| 74  | 3L    | 40     | THR  |
| 74  | 3L    | 45     | THR  |
| 74  | 3L    | 67     | ASP  |
| 74  | 3L    | 91     | THR  |
| 74  | 3L    | 113    | GLN  |
| 74  | 3L    | 133    | THR  |
| 75  | 3M    | 2      | VAL  |
| 75  | 3M    | 6      | VAL  |
| 75  | 3M    | 13     | SER  |
| 75  | 3M    | 26     | LEU  |
| 75  | 3M    | 35     | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | 3M    | 76  | SER  |
| 75  | 3M    | 104 | LEU  |
| 75  | 3M    | 121 | THR  |
| 76  | 3N    | 5   | VAL  |
| 76  | 3N    | 14  | THR  |
| 76  | 3N    | 35  | VAL  |
| 76  | 3N    | 50  | THR  |
| 76  | 3N    | 57  | VAL  |
| 77  | 3O    | 46  | ASN  |
| 77  | 3O    | 48  | VAL  |
| 77  | 3O    | 62  | VAL  |
| 77  | 3O    | 69  | THR  |
| 77  | 3O    | 77  | LEU  |
| 77  | 3O    | 79  | ILE  |
| 77  | 3O    | 98  | LYS  |
| 77  | 3O    | 110 | THR  |
| 77  | 3O    | 112 | ASN  |
| 78  | 3P    | 3   | LEU  |
| 78  | 3P    | 17  | ARG  |
| 78  | 3P    | 43  | ILE  |
| 78  | 3P    | 44  | THR  |
| 78  | 3P    | 61  | THR  |
| 78  | 3P    | 62  | VAL  |
| 79  | 3Q    | 6   | LEU  |
| 79  | 3Q    | 11  | LYS  |
| 79  | 3Q    | 27  | LYS  |
| 79  | 3Q    | 46  | VAL  |
| 80  | 3R    | 98  | VAL  |
| 80  | 3R    | 102 | VAL  |
| 80  | 3R    | 147 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1D    | 8   | GLN  |
| 4   | 1D    | 22  | HIS  |
| 4   | 1D    | 83  | HIS  |
| 4   | 1D    | 95  | GLN  |
| 4   | 1D    | 205 | ASN  |
| 6   | 1F    | 43  | ASN  |
| 6   | 1F    | 198 | ASN  |
| 6   | 1F    | 317 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 1F    | 329 | ASN  |
| 6   | 1F    | 347 | HIS  |
| 7   | 1G    | 244 | HIS  |
| 7   | 1G    | 267 | ASN  |
| 7   | 1G    | 291 | GLN  |
| 8   | 1H    | 205 | ASN  |
| 8   | 1H    | 245 | GLN  |
| 9   | 2A    | 39  | GLN  |
| 10  | 2B    | 64  | GLN  |
| 10  | 2B    | 153 | GLN  |
| 10  | 2B    | 195 | HIS  |
| 11  | 2C    | 39  | ASN  |
| 13  | 2E    | 10  | ASN  |
| 13  | 2E    | 42  | GLN  |
| 14  | 2F    | 19  | GLN  |
| 14  | 2F    | 149 | GLN  |
| 15  | 2G    | 20  | HIS  |
| 16  | 2H    | 109 | HIS  |
| 16  | 2H    | 145 | ASN  |
| 16  | 2H    | 201 | HIS  |
| 17  | 2I    | 50  | ASN  |
| 17  | 2I    | 63  | ASN  |
| 17  | 2I    | 184 | ASN  |
| 18  | 2J    | 137 | ASN  |
| 19  | 2K    | 188 | ASN  |
| 20  | 2L    | 178 | GLN  |
| 21  | 2M    | 23  | HIS  |
| 23  | 2O    | 41  | GLN  |
| 23  | 2O    | 94  | ASN  |
| 24  | 2P    | 77  | HIS  |
| 25  | 2Q    | 45  | ASN  |
| 26  | 2R    | 57  | GLN  |
| 26  | 2R    | 107 | HIS  |
| 27  | 2S    | 14  | ASN  |
| 29  | 2U    | 19  | HIS  |
| 29  | 2U    | 60  | HIS  |
| 30  | 2V    | 6   | ASN  |
| 30  | 2V    | 58  | GLN  |
| 31  | 2W    | 33  | GLN  |
| 32  | 2X    | 18  | ASN  |
| 32  | 2X    | 28  | ASN  |
| 32  | 2X    | 116 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2a    | 3   | GLN  |
| 35  | 2a    | 110 | GLN  |
| 36  | 2b    | 65  | GLN  |
| 40  | 2f    | 33  | ASN  |
| 43  | 2i    | 19  | GLN  |
| 44  | 2j    | 72  | ASN  |
| 45  | 2k    | 4   | HIS  |
| 46  | 2l    | 19  | HIS  |
| 46  | 2l    | 94  | ASN  |
| 48  | 2n    | 36  | GLN  |
| 48  | 2n    | 113 | GLN  |
| 48  | 2n    | 132 | GLN  |
| 48  | 2n    | 165 | ASN  |
| 49  | 2o    | 75  | GLN  |
| 49  | 2o    | 118 | GLN  |
| 49  | 2o    | 147 | ASN  |
| 51  | 2q    | 36  | HIS  |
| 51  | 2q    | 50  | ASN  |
| 51  | 2q    | 188 | ASN  |
| 51  | 2q    | 197 | ASN  |
| 52  | 2r    | 114 | ASN  |
| 52  | 2r    | 203 | ASN  |
| 53  | 2s    | 126 | HIS  |
| 54  | 2t    | 88  | ASN  |
| 55  | 2u    | 50  | GLN  |
| 56  | 2v    | 11  | GLN  |
| 56  | 2v    | 19  | ASN  |
| 57  | 2w    | 104 | GLN  |
| 59  | 2y    | 29  | HIS  |
| 60  | 2z    | 73  | ASN  |
| 60  | 2z    | 101 | ASN  |
| 61  | 20    | 63  | HIS  |
| 64  | 3B    | 73  | GLN  |
| 64  | 3B    | 87  | ASN  |
| 68  | 3F    | 222 | ASN  |
| 68  | 3F    | 237 | ASN  |
| 71  | 3I    | 140 | GLN  |
| 71  | 3I    | 156 | HIS  |
| 73  | 3K    | 5   | HIS  |
| 73  | 3K    | 13  | GLN  |
| 74  | 3L    | 20  | GLN  |
| 76  | 3N    | 22  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 76  | 3N    | 106 | GLN  |
| 78  | 3P    | 26  | GLN  |
| 78  | 3P    | 51  | GLN  |
| 80  | 3R    | 93  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 3704/5070 (73%) | 810 (21%)         | 54 (1%)         |
| 2   | 1B    | 119/121 (98%)   | 14 (11%)          | 2 (1%)          |
| 3   | 1C    | 155/157 (98%)   | 28 (18%)          | 2 (1%)          |
| 47  | 2m    | 1714/1869 (91%) | 492 (28%)         | 0               |
| All | All   | 5692/7217 (78%) | 1344 (23%)        | 58 (1%)         |

All (1344) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 6   | C    |
| 1   | 1A    | 13  | U    |
| 1   | 1A    | 39  | A    |
| 1   | 1A    | 42  | A    |
| 1   | 1A    | 48  | G    |
| 1   | 1A    | 59  | A    |
| 1   | 1A    | 64  | A    |
| 1   | 1A    | 65  | A    |
| 1   | 1A    | 66  | A    |
| 1   | 1A    | 67  | C    |
| 1   | 1A    | 73  | A    |
| 1   | 1A    | 91  | G    |
| 1   | 1A    | 98  | A    |
| 1   | 1A    | 104 | G    |
| 1   | 1A    | 109 | G    |
| 1   | 1A    | 110 | C    |
| 1   | 1A    | 119 | G    |
| 1   | 1A    | 120 | A    |
| 1   | 1A    | 121 | A    |
| 1   | 1A    | 122 | U    |
| 1   | 1A    | 128 | C    |
| 1   | 1A    | 130 | C    |
| 1   | 1A    | 131 | C    |
| 1   | 1A    | 133 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 135 | G    |
| 1   | 1A    | 136 | C    |
| 1   | 1A    | 137 | G    |
| 1   | 1A    | 144 | G    |
| 1   | 1A    | 159 | C    |
| 1   | 1A    | 171 | U    |
| 1   | 1A    | 172 | C    |
| 1   | 1A    | 179 | G    |
| 1   | 1A    | 180 | C    |
| 1   | 1A    | 183 | C    |
| 1   | 1A    | 184 | U    |
| 1   | 1A    | 185 | C    |
| 1   | 1A    | 188 | G    |
| 1   | 1A    | 189 | G    |
| 1   | 1A    | 197 | A    |
| 1   | 1A    | 200 | U    |
| 1   | 1A    | 201 | C    |
| 1   | 1A    | 209 | U    |
| 1   | 1A    | 216 | C    |
| 1   | 1A    | 217 | C    |
| 1   | 1A    | 218 | A    |
| 1   | 1A    | 219 | G    |
| 1   | 1A    | 227 | A    |
| 1   | 1A    | 233 | U    |
| 1   | 1A    | 234 | G    |
| 1   | 1A    | 265 | C    |
| 1   | 1A    | 266 | C    |
| 1   | 1A    | 275 | C    |
| 1   | 1A    | 278 | G    |
| 1   | 1A    | 280 | G    |
| 1   | 1A    | 295 | A    |
| 1   | 1A    | 297 | U    |
| 1   | 1A    | 306 | A    |
| 1   | 1A    | 315 | G    |
| 1   | 1A    | 316 | U    |
| 1   | 1A    | 340 | C    |
| 1   | 1A    | 384 | A    |
| 1   | 1A    | 386 | A    |
| 1   | 1A    | 387 | G    |
| 1   | 1A    | 396 | A    |
| 1   | 1A    | 407 | A    |
| 1   | 1A    | 409 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 410 | A    |
| 1   | 1A    | 412 | G    |
| 1   | 1A    | 413 | G    |
| 1   | 1A    | 414 | C    |
| 1   | 1A    | 415 | G    |
| 1   | 1A    | 417 | G    |
| 1   | 1A    | 418 | A    |
| 1   | 1A    | 449 | C    |
| 1   | 1A    | 450 | G    |
| 1   | 1A    | 452 | A    |
| 1   | 1A    | 453 | G    |
| 1   | 1A    | 456 | C    |
| 1   | 1A    | 457 | G    |
| 1   | 1A    | 467 | U    |
| 1   | 1A    | 484 | U    |
| 1   | 1A    | 485 | C    |
| 1   | 1A    | 486 | C    |
| 1   | 1A    | 493 | G    |
| 1   | 1A    | 494 | U    |
| 1   | 1A    | 497 | G    |
| 1   | 1A    | 498 | C    |
| 1   | 1A    | 500 | G    |
| 1   | 1A    | 502 | C    |
| 1   | 1A    | 503 | C    |
| 1   | 1A    | 504 | G    |
| 1   | 1A    | 505 | G    |
| 1   | 1A    | 507 | G    |
| 1   | 1A    | 509 | A    |
| 1   | 1A    | 510 | U    |
| 1   | 1A    | 512 | U    |
| 1   | 1A    | 513 | U    |
| 1   | 1A    | 514 | U    |
| 1   | 1A    | 517 | C    |
| 1   | 1A    | 518 | G    |
| 1   | 1A    | 643 | C    |
| 1   | 1A    | 644 | G    |
| 1   | 1A    | 645 | G    |
| 1   | 1A    | 646 | G    |
| 1   | 1A    | 654 | C    |
| 1   | 1A    | 657 | C    |
| 1   | 1A    | 665 | C    |
| 1   | 1A    | 666 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 667 | A    |
| 1   | 1A    | 668 | C    |
| 1   | 1A    | 673 | C    |
| 1   | 1A    | 685 | C    |
| 1   | 1A    | 686 | A    |
| 1   | 1A    | 687 | U    |
| 1   | 1A    | 696 | C    |
| 1   | 1A    | 703 | G    |
| 1   | 1A    | 704 | C    |
| 1   | 1A    | 706 | C    |
| 1   | 1A    | 731 | G    |
| 1   | 1A    | 738 | C    |
| 1   | 1A    | 739 | G    |
| 1   | 1A    | 740 | G    |
| 1   | 1A    | 742 | G    |
| 1   | 1A    | 744 | G    |
| 1   | 1A    | 753 | C    |
| 1   | 1A    | 754 | U    |
| 1   | 1A    | 904 | C    |
| 1   | 1A    | 905 | C    |
| 1   | 1A    | 913 | U    |
| 1   | 1A    | 914 | U    |
| 1   | 1A    | 915 | A    |
| 1   | 1A    | 916 | C    |
| 1   | 1A    | 917 | A    |
| 1   | 1A    | 923 | C    |
| 1   | 1A    | 924 | C    |
| 1   | 1A    | 925 | C    |
| 1   | 1A    | 926 | G    |
| 1   | 1A    | 932 | A    |
| 1   | 1A    | 933 | G    |
| 1   | 1A    | 936 | C    |
| 1   | 1A    | 944 | A    |
| 1   | 1A    | 945 | U    |
| 1   | 1A    | 959 | G    |
| 1   | 1A    | 960 | A    |
| 1   | 1A    | 961 | G    |
| 1   | 1A    | 962 | C    |
| 1   | 1A    | 965 | G    |
| 1   | 1A    | 966 | A    |
| 1   | 1A    | 967 | C    |
| 1   | 1A    | 969 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 970  | G    |
| 1   | 1A    | 971  | U    |
| 1   | 1A    | 977  | C    |
| 1   | 1A    | 982  | U    |
| 1   | 1A    | 984  | C    |
| 1   | 1A    | 989  | U    |
| 1   | 1A    | 990  | C    |
| 1   | 1A    | 991  | C    |
| 1   | 1A    | 992  | C    |
| 1   | 1A    | 993  | G    |
| 1   | 1A    | 995  | C    |
| 1   | 1A    | 1048 | G    |
| 1   | 1A    | 1049 | C    |
| 1   | 1A    | 1051 | G    |
| 1   | 1A    | 1066 | G    |
| 1   | 1A    | 1070 | G    |
| 1   | 1A    | 1071 | C    |
| 1   | 1A    | 1072 | C    |
| 1   | 1A    | 1075 | G    |
| 1   | 1A    | 1079 | C    |
| 1   | 1A    | 1082 | C    |
| 1   | 1A    | 1168 | G    |
| 1   | 1A    | 1172 | C    |
| 1   | 1A    | 1173 | G    |
| 1   | 1A    | 1174 | G    |
| 1   | 1A    | 1178 | G    |
| 1   | 1A    | 1179 | U    |
| 1   | 1A    | 1180 | C    |
| 1   | 1A    | 1181 | C    |
| 1   | 1A    | 1182 | C    |
| 1   | 1A    | 1183 | C    |
| 1   | 1A    | 1184 | A    |
| 1   | 1A    | 1198 | G    |
| 1   | 1A    | 1202 | C    |
| 1   | 1A    | 1203 | G    |
| 1   | 1A    | 1211 | G    |
| 1   | 1A    | 1215 | C    |
| 1   | 1A    | 1216 | C    |
| 1   | 1A    | 1217 | G    |
| 1   | 1A    | 1218 | G    |
| 1   | 1A    | 1219 | G    |
| 1   | 1A    | 1220 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1221 | G    |
| 1   | 1A    | 1222 | A    |
| 1   | 1A    | 1235 | G    |
| 1   | 1A    | 1241 | C    |
| 1   | 1A    | 1242 | G    |
| 1   | 1A    | 1253 | G    |
| 1   | 1A    | 1254 | A    |
| 1   | 1A    | 1255 | A    |
| 1   | 1A    | 1263 | A    |
| 1   | 1A    | 1266 | G    |
| 1   | 1A    | 1269 | G    |
| 1   | 1A    | 1270 | A    |
| 1   | 1A    | 1271 | G    |
| 1   | 1A    | 1272 | C    |
| 1   | 1A    | 1273 | G    |
| 1   | 1A    | 1275 | G    |
| 1   | 1A    | 1280 | C    |
| 1   | 1A    | 1284 | G    |
| 1   | 1A    | 1285 | U    |
| 1   | 1A    | 1287 | G    |
| 1   | 1A    | 1293 | G    |
| 1   | 1A    | 1294 | A    |
| 1   | 1A    | 1296 | G    |
| 1   | 1A    | 1301 | C    |
| 1   | 1A    | 1302 | U    |
| 1   | 1A    | 1303 | A    |
| 1   | 1A    | 1313 | C    |
| 1   | 1A    | 1326 | A    |
| 1   | 1A    | 1337 | A    |
| 1   | 1A    | 1338 | G    |
| 1   | 1A    | 1354 | A    |
| 1   | 1A    | 1358 | G    |
| 1   | 1A    | 1359 | G    |
| 1   | 1A    | 1365 | C    |
| 1   | 1A    | 1366 | G    |
| 1   | 1A    | 1367 | C    |
| 1   | 1A    | 1378 | C    |
| 1   | 1A    | 1387 | A    |
| 1   | 1A    | 1393 | G    |
| 1   | 1A    | 1394 | G    |
| 1   | 1A    | 1397 | A    |
| 1   | 1A    | 1398 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1399 | G    |
| 1   | 1A    | 1405 | C    |
| 1   | 1A    | 1409 | C    |
| 1   | 1A    | 1410 | U    |
| 1   | 1A    | 1411 | C    |
| 1   | 1A    | 1420 | A    |
| 1   | 1A    | 1437 | C    |
| 1   | 1A    | 1439 | C    |
| 1   | 1A    | 1441 | C    |
| 1   | 1A    | 1443 | A    |
| 1   | 1A    | 1444 | G    |
| 1   | 1A    | 1446 | C    |
| 1   | 1A    | 1447 | C    |
| 1   | 1A    | 1482 | G    |
| 1   | 1A    | 1483 | C    |
| 1   | 1A    | 1498 | G    |
| 1   | 1A    | 1502 | G    |
| 1   | 1A    | 1504 | G    |
| 1   | 1A    | 1534 | A    |
| 1   | 1A    | 1547 | A    |
| 1   | 1A    | 1564 | A    |
| 1   | 1A    | 1566 | C    |
| 1   | 1A    | 1578 | U    |
| 1   | 1A    | 1591 | U    |
| 1   | 1A    | 1596 | U    |
| 1   | 1A    | 1613 | A    |
| 1   | 1A    | 1624 | G    |
| 1   | 1A    | 1625 | G    |
| 1   | 1A    | 1631 | A    |
| 1   | 1A    | 1633 | G    |
| 1   | 1A    | 1634 | A    |
| 1   | 1A    | 1638 | A    |
| 1   | 1A    | 1640 | C    |
| 1   | 1A    | 1642 | A    |
| 1   | 1A    | 1654 | G    |
| 1   | 1A    | 1661 | C    |
| 1   | 1A    | 1663 | C    |
| 1   | 1A    | 1676 | C    |
| 1   | 1A    | 1677 | U    |
| 1   | 1A    | 1691 | G    |
| 1   | 1A    | 1697 | G    |
| 1   | 1A    | 1699 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1700 | G    |
| 1   | 1A    | 1703 | C    |
| 1   | 1A    | 1704 | C    |
| 1   | 1A    | 1705 | G    |
| 1   | 1A    | 1707 | C    |
| 1   | 1A    | 1708 | G    |
| 1   | 1A    | 1729 | A    |
| 1   | 1A    | 1731 | C    |
| 1   | 1A    | 1740 | C    |
| 1   | 1A    | 1742 | A    |
| 1   | 1A    | 1757 | U    |
| 1   | 1A    | 1758 | G    |
| 1   | 1A    | 1759 | G    |
| 1   | 1A    | 1761 | G    |
| 1   | 1A    | 1762 | C    |
| 1   | 1A    | 1763 | C    |
| 1   | 1A    | 1764 | G    |
| 1   | 1A    | 1765 | A    |
| 1   | 1A    | 1766 | A    |
| 1   | 1A    | 1768 | C    |
| 1   | 1A    | 1769 | G    |
| 1   | 1A    | 1770 | A    |
| 1   | 1A    | 1775 | A    |
| 1   | 1A    | 1787 | A    |
| 1   | 1A    | 1804 | A    |
| 1   | 1A    | 1805 | A    |
| 1   | 1A    | 1810 | G    |
| 1   | 1A    | 1820 | C    |
| 1   | 1A    | 1821 | G    |
| 1   | 1A    | 1822 | U    |
| 1   | 1A    | 1834 | U    |
| 1   | 1A    | 1836 | G    |
| 1   | 1A    | 1837 | A    |
| 1   | 1A    | 1842 | G    |
| 1   | 1A    | 1855 | G    |
| 1   | 1A    | 1869 | G    |
| 1   | 1A    | 1897 | A    |
| 1   | 1A    | 1918 | U    |
| 1   | 1A    | 1919 | G    |
| 1   | 1A    | 1920 | C    |
| 1   | 1A    | 1921 | C    |
| 1   | 1A    | 1922 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1925 | G    |
| 1   | 1A    | 1931 | C    |
| 1   | 1A    | 1932 | A    |
| 1   | 1A    | 1940 | G    |
| 1   | 1A    | 1948 | G    |
| 1   | 1A    | 1959 | U    |
| 1   | 1A    | 1960 | A    |
| 1   | 1A    | 1961 | G    |
| 1   | 1A    | 1962 | A    |
| 1   | 1A    | 1966 | C    |
| 1   | 1A    | 1968 | G    |
| 1   | 1A    | 1974 | U    |
| 1   | 1A    | 1975 | G    |
| 1   | 1A    | 1978 | C    |
| 1   | 1A    | 1980 | U    |
| 1   | 1A    | 1981 | G    |
| 1   | 1A    | 1982 | G    |
| 1   | 1A    | 1983 | A    |
| 1   | 1A    | 1984 | A    |
| 1   | 1A    | 1985 | G    |
| 1   | 1A    | 1987 | C    |
| 1   | 1A    | 1988 | G    |
| 1   | 1A    | 1991 | A    |
| 1   | 1A    | 1993 | C    |
| 1   | 1A    | 1995 | G    |
| 1   | 1A    | 1996 | C    |
| 1   | 1A    | 1998 | A    |
| 1   | 1A    | 1999 | A    |
| 1   | 1A    | 2001 | G    |
| 1   | 1A    | 2002 | A    |
| 1   | 1A    | 2003 | G    |
| 1   | 1A    | 2004 | U    |
| 1   | 1A    | 2005 | G    |
| 1   | 1A    | 2006 | U    |
| 1   | 1A    | 2007 | G    |
| 1   | 1A    | 2009 | A    |
| 1   | 1A    | 2010 | A    |
| 1   | 1A    | 2011 | C    |
| 1   | 1A    | 2012 | A    |
| 1   | 1A    | 2013 | A    |
| 1   | 1A    | 2015 | U    |
| 1   | 1A    | 2016 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2018 | C    |
| 1   | 1A    | 2019 | C    |
| 1   | 1A    | 2020 | U    |
| 1   | 1A    | 2021 | G    |
| 1   | 1A    | 2024 | G    |
| 1   | 1A    | 2025 | A    |
| 1   | 1A    | 2026 | A    |
| 1   | 1A    | 2034 | G    |
| 1   | 1A    | 2046 | G    |
| 1   | 1A    | 2048 | U    |
| 1   | 1A    | 2055 | G    |
| 1   | 1A    | 2056 | G    |
| 1   | 1A    | 2069 | A    |
| 1   | 1A    | 2084 | C    |
| 1   | 1A    | 2089 | G    |
| 1   | 1A    | 2092 | G    |
| 1   | 1A    | 2093 | A    |
| 1   | 1A    | 2094 | G    |
| 1   | 1A    | 2095 | A    |
| 1   | 1A    | 2097 | U    |
| 1   | 1A    | 2098 | G    |
| 1   | 1A    | 2101 | C    |
| 1   | 1A    | 2102 | G    |
| 1   | 1A    | 2103 | G    |
| 1   | 1A    | 2111 | G    |
| 1   | 1A    | 2112 | G    |
| 1   | 1A    | 2113 | C    |
| 1   | 1A    | 2250 | C    |
| 1   | 1A    | 2252 | G    |
| 1   | 1A    | 2253 | A    |
| 1   | 1A    | 2256 | C    |
| 1   | 1A    | 2257 | C    |
| 1   | 1A    | 2258 | C    |
| 1   | 1A    | 2259 | G    |
| 1   | 1A    | 2261 | G    |
| 1   | 1A    | 2268 | A    |
| 1   | 1A    | 2289 | C    |
| 1   | 1A    | 2300 | A    |
| 1   | 1A    | 2301 | G    |
| 1   | 1A    | 2306 | G    |
| 1   | 1A    | 2313 | A    |
| 1   | 1A    | 2333 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2348 | G    |
| 1   | 1A    | 2351 | C    |
| 1   | 1A    | 2360 | A    |
| 1   | 1A    | 2370 | A    |
| 1   | 1A    | 2390 | G    |
| 1   | 1A    | 2395 | A    |
| 1   | 1A    | 2397 | G    |
| 1   | 1A    | 2417 | A    |
| 1   | 1A    | 2421 | G    |
| 1   | 1A    | 2428 | A    |
| 1   | 1A    | 2441 | C    |
| 1   | 1A    | 2460 | A    |
| 1   | 1A    | 2461 | G    |
| 1   | 1A    | 2465 | C    |
| 1   | 1A    | 2469 | C    |
| 1   | 1A    | 2470 | C    |
| 1   | 1A    | 2471 | G    |
| 1   | 1A    | 2474 | G    |
| 1   | 1A    | 2475 | G    |
| 1   | 1A    | 2483 | G    |
| 1   | 1A    | 2484 | A    |
| 1   | 1A    | 2485 | U    |
| 1   | 1A    | 2487 | G    |
| 1   | 1A    | 2488 | C    |
| 1   | 1A    | 2490 | U    |
| 1   | 1A    | 2491 | C    |
| 1   | 1A    | 2493 | G    |
| 1   | 1A    | 2495 | U    |
| 1   | 1A    | 2496 | G    |
| 1   | 1A    | 2498 | C    |
| 1   | 1A    | 2503 | G    |
| 1   | 1A    | 2504 | C    |
| 1   | 1A    | 2505 | C    |
| 1   | 1A    | 2506 | G    |
| 1   | 1A    | 2512 | A    |
| 1   | 1A    | 2513 | A    |
| 1   | 1A    | 2529 | A    |
| 1   | 1A    | 2530 | U    |
| 1   | 1A    | 2537 | A    |
| 1   | 1A    | 2544 | G    |
| 1   | 1A    | 2546 | G    |
| 1   | 1A    | 2547 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2553 | A    |
| 1   | 1A    | 2554 | U    |
| 1   | 1A    | 2555 | G    |
| 1   | 1A    | 2556 | G    |
| 1   | 1A    | 2560 | C    |
| 1   | 1A    | 2561 | C    |
| 1   | 1A    | 2563 | C    |
| 1   | 1A    | 2564 | G    |
| 1   | 1A    | 2566 | G    |
| 1   | 1A    | 2569 | G    |
| 1   | 1A    | 2583 | C    |
| 1   | 1A    | 2586 | G    |
| 1   | 1A    | 2587 | A    |
| 1   | 1A    | 2589 | C    |
| 1   | 1A    | 2601 | A    |
| 1   | 1A    | 2602 | G    |
| 1   | 1A    | 2618 | G    |
| 1   | 1A    | 2638 | G    |
| 1   | 1A    | 2640 | G    |
| 1   | 1A    | 2653 | C    |
| 1   | 1A    | 2662 | G    |
| 1   | 1A    | 2669 | C    |
| 1   | 1A    | 2670 | C    |
| 1   | 1A    | 2676 | A    |
| 1   | 1A    | 2679 | G    |
| 1   | 1A    | 2687 | U    |
| 1   | 1A    | 2695 | A    |
| 1   | 1A    | 2696 | A    |
| 1   | 1A    | 2708 | U    |
| 1   | 1A    | 2710 | C    |
| 1   | 1A    | 2711 | G    |
| 1   | 1A    | 2712 | G    |
| 1   | 1A    | 2725 | A    |
| 1   | 1A    | 2726 | G    |
| 1   | 1A    | 2739 | C    |
| 1   | 1A    | 2743 | A    |
| 1   | 1A    | 2759 | G    |
| 1   | 1A    | 2761 | U    |
| 1   | 1A    | 2762 | G    |
| 1   | 1A    | 2763 | U    |
| 1   | 1A    | 2767 | U    |
| 1   | 1A    | 2768 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2769 | U    |
| 1   | 1A    | 2770 | C    |
| 1   | 1A    | 2776 | G    |
| 1   | 1A    | 2787 | A    |
| 1   | 1A    | 2788 | U    |
| 1   | 1A    | 2790 | U    |
| 1   | 1A    | 2794 | C    |
| 1   | 1A    | 2797 | C    |
| 1   | 1A    | 2798 | A    |
| 1   | 1A    | 2814 | C    |
| 1   | 1A    | 2826 | U    |
| 1   | 1A    | 2827 | G    |
| 1   | 1A    | 2829 | U    |
| 1   | 1A    | 2855 | G    |
| 1   | 1A    | 2860 | C    |
| 1   | 1A    | 2870 | A    |
| 1   | 1A    | 2875 | C    |
| 1   | 1A    | 2877 | G    |
| 1   | 1A    | 2905 | C    |
| 1   | 1A    | 2906 | G    |
| 1   | 1A    | 2908 | U    |
| 1   | 1A    | 3585 | G    |
| 1   | 1A    | 3586 | G    |
| 1   | 1A    | 3588 | C    |
| 1   | 1A    | 3591 | C    |
| 1   | 1A    | 3592 | G    |
| 1   | 1A    | 3593 | C    |
| 1   | 1A    | 3595 | U    |
| 1   | 1A    | 3596 | A    |
| 1   | 1A    | 3597 | G    |
| 1   | 1A    | 3605 | C    |
| 1   | 1A    | 3617 | G    |
| 1   | 1A    | 3626 | G    |
| 1   | 1A    | 3635 | A    |
| 1   | 1A    | 3642 | A    |
| 1   | 1A    | 3644 | U    |
| 1   | 1A    | 3646 | A    |
| 1   | 1A    | 3648 | A    |
| 1   | 1A    | 3662 | A    |
| 1   | 1A    | 3664 | G    |
| 1   | 1A    | 3670 | C    |
| 1   | 1A    | 3671 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 3673 | C    |
| 1   | 1A    | 3696 | C    |
| 1   | 1A    | 3710 | G    |
| 1   | 1A    | 3711 | A    |
| 1   | 1A    | 3712 | A    |
| 1   | 1A    | 3713 | U    |
| 1   | 1A    | 3714 | G    |
| 1   | 1A    | 3727 | A    |
| 1   | 1A    | 3728 | A    |
| 1   | 1A    | 3748 | A    |
| 1   | 1A    | 3753 | G    |
| 1   | 1A    | 3758 | U    |
| 1   | 1A    | 3760 | A    |
| 1   | 1A    | 3761 | C    |
| 1   | 1A    | 3763 | A    |
| 1   | 1A    | 3769 | C    |
| 1   | 1A    | 3771 | C    |
| 1   | 1A    | 3773 | U    |
| 1   | 1A    | 3774 | A    |
| 1   | 1A    | 3776 | G    |
| 1   | 1A    | 3777 | G    |
| 1   | 1A    | 3783 | A    |
| 1   | 1A    | 3784 | A    |
| 1   | 1A    | 3785 | A    |
| 1   | 1A    | 3786 | U    |
| 1   | 1A    | 3811 | G    |
| 1   | 1A    | 3817 | A    |
| 1   | 1A    | 3818 | U    |
| 1   | 1A    | 3819 | G    |
| 1   | 1A    | 3838 | U    |
| 1   | 1A    | 3839 | G    |
| 1   | 1A    | 3840 | U    |
| 1   | 1A    | 3867 | A    |
| 1   | 1A    | 3869 | C    |
| 1   | 1A    | 3874 | G    |
| 1   | 1A    | 3877 | A    |
| 1   | 1A    | 3878 | C    |
| 1   | 1A    | 3879 | G    |
| 1   | 1A    | 3885 | G    |
| 1   | 1A    | 3889 | G    |
| 1   | 1A    | 3897 | G    |
| 1   | 1A    | 3898 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 3901 | A    |
| 1   | 1A    | 3905 | A    |
| 1   | 1A    | 3906 | A    |
| 1   | 1A    | 3907 | G    |
| 1   | 1A    | 3908 | A    |
| 1   | 1A    | 3915 | U    |
| 1   | 1A    | 3922 | G    |
| 1   | 1A    | 3923 | A    |
| 1   | 1A    | 3937 | C    |
| 1   | 1A    | 3938 | G    |
| 1   | 1A    | 3939 | G    |
| 1   | 1A    | 3942 | A    |
| 1   | 1A    | 3947 | A    |
| 1   | 1A    | 3948 | C    |
| 1   | 1A    | 3950 | U    |
| 1   | 1A    | 3951 | G    |
| 1   | 1A    | 3952 | A    |
| 1   | 1A    | 3954 | A    |
| 1   | 1A    | 3955 | G    |
| 1   | 1A    | 3956 | G    |
| 1   | 1A    | 3957 | U    |
| 1   | 1A    | 3958 | G    |
| 1   | 1A    | 3959 | U    |
| 1   | 1A    | 3960 | A    |
| 1   | 1A    | 3961 | G    |
| 1   | 1A    | 3962 | A    |
| 1   | 1A    | 3963 | A    |
| 1   | 1A    | 3964 | U    |
| 1   | 1A    | 3965 | A    |
| 1   | 1A    | 3966 | A    |
| 1   | 1A    | 3968 | U    |
| 1   | 1A    | 3970 | G    |
| 1   | 1A    | 3973 | G    |
| 1   | 1A    | 3975 | C    |
| 1   | 1A    | 4035 | G    |
| 1   | 1A    | 4036 | G    |
| 1   | 1A    | 4038 | C    |
| 1   | 1A    | 4039 | G    |
| 1   | 1A    | 4041 | C    |
| 1   | 1A    | 4042 | G    |
| 1   | 1A    | 4043 | G    |
| 1   | 1A    | 4044 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 4046 | A    |
| 1   | 1A    | 4048 | A    |
| 1   | 1A    | 4049 | U    |
| 1   | 1A    | 4051 | C    |
| 1   | 1A    | 4053 | A    |
| 1   | 1A    | 4054 | C    |
| 1   | 1A    | 4055 | U    |
| 1   | 1A    | 4056 | A    |
| 1   | 1A    | 4057 | C    |
| 1   | 1A    | 4059 | C    |
| 1   | 1A    | 4061 | G    |
| 1   | 1A    | 4064 | C    |
| 1   | 1A    | 4065 | G    |
| 1   | 1A    | 4066 | U    |
| 1   | 1A    | 4076 | G    |
| 1   | 1A    | 4084 | G    |
| 1   | 1A    | 4086 | G    |
| 1   | 1A    | 4088 | C    |
| 1   | 1A    | 4099 | G    |
| 1   | 1A    | 4100 | C    |
| 1   | 1A    | 4101 | C    |
| 1   | 1A    | 4102 | C    |
| 1   | 1A    | 4104 | G    |
| 1   | 1A    | 4105 | A    |
| 1   | 1A    | 4106 | G    |
| 1   | 1A    | 4107 | G    |
| 1   | 1A    | 4108 | G    |
| 1   | 1A    | 4109 | G    |
| 1   | 1A    | 4110 | C    |
| 1   | 1A    | 4111 | U    |
| 1   | 1A    | 4112 | C    |
| 1   | 1A    | 4114 | C    |
| 1   | 1A    | 4115 | G    |
| 1   | 1A    | 4116 | C    |
| 1   | 1A    | 4119 | C    |
| 1   | 1A    | 4120 | U    |
| 1   | 1A    | 4121 | G    |
| 1   | 1A    | 4122 | G    |
| 1   | 1A    | 4127 | A    |
| 1   | 1A    | 4141 | G    |
| 1   | 1A    | 4142 | C    |
| 1   | 1A    | 4143 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 4144 | C    |
| 1   | 1A    | 4154 | G    |
| 1   | 1A    | 4162 | C    |
| 1   | 1A    | 4163 | U    |
| 1   | 1A    | 4168 | G    |
| 1   | 1A    | 4170 | A    |
| 1   | 1A    | 4183 | G    |
| 1   | 1A    | 4184 | G    |
| 1   | 1A    | 4191 | G    |
| 1   | 1A    | 4201 | G    |
| 1   | 1A    | 4203 | A    |
| 1   | 1A    | 4204 | C    |
| 1   | 1A    | 4214 | A    |
| 1   | 1A    | 4229 | U    |
| 1   | 1A    | 4233 | A    |
| 1   | 1A    | 4251 | A    |
| 1   | 1A    | 4254 | G    |
| 1   | 1A    | 4256 | A    |
| 1   | 1A    | 4268 | A    |
| 1   | 1A    | 4273 | A    |
| 1   | 1A    | 4280 | A    |
| 1   | 1A    | 4288 | C    |
| 1   | 1A    | 4291 | G    |
| 1   | 1A    | 4305 | G    |
| 1   | 1A    | 4306 | U    |
| 1   | 1A    | 4314 | C    |
| 1   | 1A    | 4318 | C    |
| 1   | 1A    | 4329 | G    |
| 1   | 1A    | 4330 | G    |
| 1   | 1A    | 4332 | C    |
| 1   | 1A    | 4337 | C    |
| 1   | 1A    | 4338 | G    |
| 1   | 1A    | 4339 | A    |
| 1   | 1A    | 4348 | A    |
| 1   | 1A    | 4349 | C    |
| 1   | 1A    | 4350 | C    |
| 1   | 1A    | 4376 | A    |
| 1   | 1A    | 4377 | G    |
| 1   | 1A    | 4378 | A    |
| 1   | 1A    | 4380 | A    |
| 1   | 1A    | 4387 | C    |
| 1   | 1A    | 4391 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 4393 | G    |
| 1   | 1A    | 4394 | A    |
| 1   | 1A    | 4420 | U    |
| 1   | 1A    | 4422 | A    |
| 1   | 1A    | 4448 | G    |
| 1   | 1A    | 4449 | A    |
| 1   | 1A    | 4453 | C    |
| 1   | 1A    | 4464 | A    |
| 1   | 1A    | 4465 | U    |
| 1   | 1A    | 4476 | C    |
| 1   | 1A    | 4500 | U    |
| 1   | 1A    | 4512 | U    |
| 1   | 1A    | 4513 | A    |
| 1   | 1A    | 4515 | G    |
| 1   | 1A    | 4519 | C    |
| 1   | 1A    | 4524 | G    |
| 1   | 1A    | 4528 | G    |
| 1   | 1A    | 4545 | G    |
| 1   | 1A    | 4548 | A    |
| 1   | 1A    | 4555 | U    |
| 1   | 1A    | 4556 | U    |
| 1   | 1A    | 4560 | C    |
| 1   | 1A    | 4567 | G    |
| 1   | 1A    | 4573 | G    |
| 1   | 1A    | 4575 | G    |
| 1   | 1A    | 4589 | A    |
| 1   | 1A    | 4590 | A    |
| 1   | 1A    | 4600 | G    |
| 1   | 1A    | 4601 | U    |
| 1   | 1A    | 4617 | G    |
| 1   | 1A    | 4636 | U    |
| 1   | 1A    | 4637 | G    |
| 1   | 1A    | 4647 | G    |
| 1   | 1A    | 4657 | U    |
| 1   | 1A    | 4670 | C    |
| 1   | 1A    | 4672 | A    |
| 1   | 1A    | 4694 | G    |
| 1   | 1A    | 4695 | C    |
| 1   | 1A    | 4700 | A    |
| 1   | 1A    | 4708 | A    |
| 1   | 1A    | 4709 | U    |
| 1   | 1A    | 4730 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 4731 | G    |
| 1   | 1A    | 4732 | G    |
| 1   | 1A    | 4737 | G    |
| 1   | 1A    | 4740 | G    |
| 1   | 1A    | 4741 | C    |
| 1   | 1A    | 4743 | G    |
| 1   | 1A    | 4744 | A    |
| 1   | 1A    | 4749 | C    |
| 1   | 1A    | 4750 | G    |
| 1   | 1A    | 4753 | U    |
| 1   | 1A    | 4754 | G    |
| 1   | 1A    | 4756 | C    |
| 1   | 1A    | 4758 | U    |
| 1   | 1A    | 4760 | G    |
| 1   | 1A    | 4764 | A    |
| 1   | 1A    | 4770 | U    |
| 1   | 1A    | 4772 | C    |
| 1   | 1A    | 4775 | C    |
| 1   | 1A    | 4776 | G    |
| 1   | 1A    | 4861 | G    |
| 1   | 1A    | 4863 | G    |
| 1   | 1A    | 4869 | U    |
| 1   | 1A    | 4871 | C    |
| 1   | 1A    | 4872 | G    |
| 1   | 1A    | 4873 | G    |
| 1   | 1A    | 4874 | A    |
| 1   | 1A    | 4875 | G    |
| 1   | 1A    | 4876 | U    |
| 1   | 1A    | 4882 | U    |
| 1   | 1A    | 4883 | C    |
| 1   | 1A    | 4884 | G    |
| 1   | 1A    | 4887 | C    |
| 1   | 1A    | 4888 | U    |
| 1   | 1A    | 4889 | G    |
| 1   | 1A    | 4890 | G    |
| 1   | 1A    | 4894 | A    |
| 1   | 1A    | 4895 | C    |
| 1   | 1A    | 4896 | G    |
| 1   | 1A    | 4897 | G    |
| 1   | 1A    | 4900 | C    |
| 1   | 1A    | 4901 | G    |
| 1   | 1A    | 4902 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 4910 | G    |
| 1   | 1A    | 4912 | G    |
| 1   | 1A    | 4914 | C    |
| 1   | 1A    | 4925 | U    |
| 1   | 1A    | 4926 | C    |
| 1   | 1A    | 4940 | C    |
| 1   | 1A    | 4941 | G    |
| 1   | 1A    | 4943 | A    |
| 1   | 1A    | 4947 | U    |
| 1   | 1A    | 4951 | G    |
| 1   | 1A    | 4955 | A    |
| 1   | 1A    | 4960 | G    |
| 1   | 1A    | 4966 | A    |
| 1   | 1A    | 4976 | U    |
| 1   | 1A    | 4988 | U    |
| 1   | 1A    | 4989 | U    |
| 1   | 1A    | 4991 | U    |
| 1   | 1A    | 5007 | A    |
| 1   | 1A    | 5014 | A    |
| 1   | 1A    | 5017 | G    |
| 1   | 1A    | 5022 | U    |
| 1   | 1A    | 5023 | C    |
| 1   | 1A    | 5024 | C    |
| 1   | 1A    | 5025 | C    |
| 1   | 1A    | 5030 | U    |
| 1   | 1A    | 5034 | A    |
| 1   | 1A    | 5041 | G    |
| 1   | 1A    | 5050 | C    |
| 1   | 1A    | 5054 | C    |
| 1   | 1A    | 5069 | U    |
| 2   | 1B    | 11   | A    |
| 2   | 1B    | 22   | A    |
| 2   | 1B    | 24   | C    |
| 2   | 1B    | 29   | C    |
| 2   | 1B    | 33   | U    |
| 2   | 1B    | 34   | C    |
| 2   | 1B    | 53   | U    |
| 2   | 1B    | 64   | G    |
| 2   | 1B    | 66   | G    |
| 2   | 1B    | 97   | G    |
| 2   | 1B    | 100  | A    |
| 2   | 1B    | 103  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1B    | 110 | G    |
| 2   | 1B    | 120 | U    |
| 3   | 1C    | 17  | A    |
| 3   | 1C    | 23  | C    |
| 3   | 1C    | 34  | U    |
| 3   | 1C    | 35  | C    |
| 3   | 1C    | 48  | A    |
| 3   | 1C    | 52  | A    |
| 3   | 1C    | 59  | A    |
| 3   | 1C    | 63  | U    |
| 3   | 1C    | 82  | A    |
| 3   | 1C    | 83  | C    |
| 3   | 1C    | 84  | A    |
| 3   | 1C    | 86  | U    |
| 3   | 1C    | 87  | G    |
| 3   | 1C    | 88  | A    |
| 3   | 1C    | 103 | A    |
| 3   | 1C    | 105 | C    |
| 3   | 1C    | 108 | A    |
| 3   | 1C    | 110 | U    |
| 3   | 1C    | 114 | G    |
| 3   | 1C    | 122 | G    |
| 3   | 1C    | 123 | U    |
| 3   | 1C    | 124 | U    |
| 3   | 1C    | 125 | C    |
| 3   | 1C    | 126 | C    |
| 3   | 1C    | 127 | U    |
| 3   | 1C    | 129 | C    |
| 3   | 1C    | 150 | C    |
| 3   | 1C    | 151 | G    |
| 47  | 2m    | 2   | A    |
| 47  | 2m    | 17  | C    |
| 47  | 2m    | 25  | A    |
| 47  | 2m    | 26  | U    |
| 47  | 2m    | 33  | G    |
| 47  | 2m    | 41  | G    |
| 47  | 2m    | 42  | A    |
| 47  | 2m    | 44  | U    |
| 47  | 2m    | 46  | A    |
| 47  | 2m    | 56  | G    |
| 47  | 2m    | 60  | A    |
| 47  | 2m    | 61  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 2m    | 64  | A    |
| 47  | 2m    | 66  | G    |
| 47  | 2m    | 67  | C    |
| 47  | 2m    | 68  | A    |
| 47  | 2m    | 70  | G    |
| 47  | 2m    | 72  | C    |
| 47  | 2m    | 73  | C    |
| 47  | 2m    | 74  | G    |
| 47  | 2m    | 75  | G    |
| 47  | 2m    | 76  | U    |
| 47  | 2m    | 77  | A    |
| 47  | 2m    | 78  | C    |
| 47  | 2m    | 79  | A    |
| 47  | 2m    | 80  | G    |
| 47  | 2m    | 103 | A    |
| 47  | 2m    | 113 | G    |
| 47  | 2m    | 115 | U    |
| 47  | 2m    | 124 | U    |
| 47  | 2m    | 125 | C    |
| 47  | 2m    | 126 | G    |
| 47  | 2m    | 127 | C    |
| 47  | 2m    | 141 | A    |
| 47  | 2m    | 143 | U    |
| 47  | 2m    | 148 | U    |
| 47  | 2m    | 155 | G    |
| 47  | 2m    | 159 | A    |
| 47  | 2m    | 161 | U    |
| 47  | 2m    | 162 | C    |
| 47  | 2m    | 167 | G    |
| 47  | 2m    | 168 | C    |
| 47  | 2m    | 173 | A    |
| 47  | 2m    | 183 | G    |
| 47  | 2m    | 184 | G    |
| 47  | 2m    | 188 | C    |
| 47  | 2m    | 190 | G    |
| 47  | 2m    | 194 | C    |
| 47  | 2m    | 198 | U    |
| 47  | 2m    | 199 | C    |
| 47  | 2m    | 206 | G    |
| 47  | 2m    | 207 | G    |
| 47  | 2m    | 208 | G    |
| 47  | 2m    | 214 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 2m    | 215 | G    |
| 47  | 2m    | 216 | C    |
| 47  | 2m    | 225 | G    |
| 47  | 2m    | 290 | U    |
| 47  | 2m    | 291 | G    |
| 47  | 2m    | 292 | A    |
| 47  | 2m    | 293 | C    |
| 47  | 2m    | 295 | C    |
| 47  | 2m    | 302 | A    |
| 47  | 2m    | 304 | C    |
| 47  | 2m    | 306 | C    |
| 47  | 2m    | 307 | G    |
| 47  | 2m    | 308 | G    |
| 47  | 2m    | 309 | G    |
| 47  | 2m    | 312 | G    |
| 47  | 2m    | 313 | A    |
| 47  | 2m    | 317 | C    |
| 47  | 2m    | 320 | G    |
| 47  | 2m    | 324 | C    |
| 47  | 2m    | 325 | C    |
| 47  | 2m    | 326 | C    |
| 47  | 2m    | 328 | U    |
| 47  | 2m    | 330 | G    |
| 47  | 2m    | 331 | C    |
| 47  | 2m    | 332 | G    |
| 47  | 2m    | 334 | C    |
| 47  | 2m    | 338 | G    |
| 47  | 2m    | 339 | A    |
| 47  | 2m    | 340 | C    |
| 47  | 2m    | 347 | G    |
| 47  | 2m    | 362 | C    |
| 47  | 2m    | 364 | A    |
| 47  | 2m    | 370 | G    |
| 47  | 2m    | 385 | G    |
| 47  | 2m    | 386 | C    |
| 47  | 2m    | 399 | C    |
| 47  | 2m    | 400 | C    |
| 47  | 2m    | 407 | G    |
| 47  | 2m    | 408 | A    |
| 47  | 2m    | 409 | C    |
| 47  | 2m    | 413 | G    |
| 47  | 2m    | 418 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 2m    | 419 | G    |
| 47  | 2m    | 438 | G    |
| 47  | 2m    | 448 | A    |
| 47  | 2m    | 450 | C    |
| 47  | 2m    | 462 | C    |
| 47  | 2m    | 465 | A    |
| 47  | 2m    | 466 | G    |
| 47  | 2m    | 471 | G    |
| 47  | 2m    | 472 | C    |
| 47  | 2m    | 473 | A    |
| 47  | 2m    | 474 | G    |
| 47  | 2m    | 482 | G    |
| 47  | 2m    | 487 | U    |
| 47  | 2m    | 488 | U    |
| 47  | 2m    | 489 | A    |
| 47  | 2m    | 492 | C    |
| 47  | 2m    | 493 | A    |
| 47  | 2m    | 503 | C    |
| 47  | 2m    | 516 | A    |
| 47  | 2m    | 532 | C    |
| 47  | 2m    | 533 | A    |
| 47  | 2m    | 534 | G    |
| 47  | 2m    | 537 | C    |
| 47  | 2m    | 538 | U    |
| 47  | 2m    | 539 | C    |
| 47  | 2m    | 540 | U    |
| 47  | 2m    | 541 | U    |
| 47  | 2m    | 542 | U    |
| 47  | 2m    | 543 | C    |
| 47  | 2m    | 544 | G    |
| 47  | 2m    | 545 | A    |
| 47  | 2m    | 547 | G    |
| 47  | 2m    | 548 | C    |
| 47  | 2m    | 549 | C    |
| 47  | 2m    | 550 | C    |
| 47  | 2m    | 551 | U    |
| 47  | 2m    | 553 | U    |
| 47  | 2m    | 554 | A    |
| 47  | 2m    | 555 | A    |
| 47  | 2m    | 556 | U    |
| 47  | 2m    | 557 | U    |
| 47  | 2m    | 559 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 2m    | 561 | A    |
| 47  | 2m    | 562 | U    |
| 47  | 2m    | 563 | G    |
| 47  | 2m    | 575 | A    |
| 47  | 2m    | 580 | U    |
| 47  | 2m    | 581 | U    |
| 47  | 2m    | 582 | C    |
| 47  | 2m    | 583 | C    |
| 47  | 2m    | 587 | A    |
| 47  | 2m    | 589 | G    |
| 47  | 2m    | 590 | A    |
| 47  | 2m    | 591 | U    |
| 47  | 2m    | 592 | C    |
| 47  | 2m    | 595 | U    |
| 47  | 2m    | 596 | U    |
| 47  | 2m    | 604 | A    |
| 47  | 2m    | 605 | A    |
| 47  | 2m    | 606 | G    |
| 47  | 2m    | 608 | C    |
| 47  | 2m    | 612 | U    |
| 47  | 2m    | 613 | G    |
| 47  | 2m    | 614 | C    |
| 47  | 2m    | 615 | C    |
| 47  | 2m    | 617 | G    |
| 47  | 2m    | 627 | U    |
| 47  | 2m    | 631 | U    |
| 47  | 2m    | 632 | C    |
| 47  | 2m    | 643 | A    |
| 47  | 2m    | 644 | G    |
| 47  | 2m    | 656 | G    |
| 47  | 2m    | 660 | C    |
| 47  | 2m    | 668 | A    |
| 47  | 2m    | 669 | A    |
| 47  | 2m    | 672 | A    |
| 47  | 2m    | 688 | U    |
| 47  | 2m    | 689 | U    |
| 47  | 2m    | 691 | G    |
| 47  | 2m    | 692 | G    |
| 47  | 2m    | 693 | A    |
| 47  | 2m    | 694 | G    |
| 47  | 2m    | 695 | C    |
| 47  | 2m    | 697 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 2m    | 698 | G    |
| 47  | 2m    | 732 | U    |
| 47  | 2m    | 733 | C    |
| 47  | 2m    | 734 | C    |
| 47  | 2m    | 735 | C    |
| 47  | 2m    | 736 | C    |
| 47  | 2m    | 738 | C    |
| 47  | 2m    | 747 | U    |
| 47  | 2m    | 748 | C    |
| 47  | 2m    | 749 | U    |
| 47  | 2m    | 751 | G    |
| 47  | 2m    | 752 | G    |
| 47  | 2m    | 753 | C    |
| 47  | 2m    | 787 | G    |
| 47  | 2m    | 788 | G    |
| 47  | 2m    | 789 | G    |
| 47  | 2m    | 793 | G    |
| 47  | 2m    | 795 | A    |
| 47  | 2m    | 796 | G    |
| 47  | 2m    | 798 | A    |
| 47  | 2m    | 799 | U    |
| 47  | 2m    | 801 | U    |
| 47  | 2m    | 810 | A    |
| 47  | 2m    | 811 | A    |
| 47  | 2m    | 812 | A    |
| 47  | 2m    | 821 | G    |
| 47  | 2m    | 822 | U    |
| 47  | 2m    | 830 | A    |
| 47  | 2m    | 834 | C    |
| 47  | 2m    | 836 | G    |
| 47  | 2m    | 837 | A    |
| 47  | 2m    | 838 | G    |
| 47  | 2m    | 839 | C    |
| 47  | 2m    | 840 | C    |
| 47  | 2m    | 842 | C    |
| 47  | 2m    | 847 | A    |
| 47  | 2m    | 848 | U    |
| 47  | 2m    | 851 | C    |
| 47  | 2m    | 869 | A    |
| 47  | 2m    | 870 | A    |
| 47  | 2m    | 873 | G    |
| 47  | 2m    | 874 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 2m    | 875 | A    |
| 47  | 2m    | 877 | C    |
| 47  | 2m    | 878 | G    |
| 47  | 2m    | 879 | C    |
| 47  | 2m    | 880 | G    |
| 47  | 2m    | 882 | U    |
| 47  | 2m    | 883 | U    |
| 47  | 2m    | 885 | U    |
| 47  | 2m    | 886 | A    |
| 47  | 2m    | 887 | U    |
| 47  | 2m    | 888 | U    |
| 47  | 2m    | 889 | U    |
| 47  | 2m    | 890 | U    |
| 47  | 2m    | 891 | G    |
| 47  | 2m    | 893 | U    |
| 47  | 2m    | 894 | G    |
| 47  | 2m    | 895 | G    |
| 47  | 2m    | 896 | U    |
| 47  | 2m    | 897 | U    |
| 47  | 2m    | 898 | U    |
| 47  | 2m    | 899 | U    |
| 47  | 2m    | 900 | C    |
| 47  | 2m    | 901 | G    |
| 47  | 2m    | 903 | A    |
| 47  | 2m    | 904 | A    |
| 47  | 2m    | 907 | G    |
| 47  | 2m    | 908 | A    |
| 47  | 2m    | 912 | C    |
| 47  | 2m    | 913 | A    |
| 47  | 2m    | 917 | U    |
| 47  | 2m    | 919 | A    |
| 47  | 2m    | 920 | A    |
| 47  | 2m    | 922 | A    |
| 47  | 2m    | 933 | G    |
| 47  | 2m    | 934 | G    |
| 47  | 2m    | 944 | A    |
| 47  | 2m    | 958 | G    |
| 47  | 2m    | 970 | G    |
| 47  | 2m    | 971 | G    |
| 47  | 2m    | 990 | A    |
| 47  | 2m    | 992 | A    |
| 47  | 2m    | 996 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | 2m    | 999  | G    |
| 47  | 2m    | 1001 | A    |
| 47  | 2m    | 1011 | A    |
| 47  | 2m    | 1012 | A    |
| 47  | 2m    | 1027 | A    |
| 47  | 2m    | 1028 | A    |
| 47  | 2m    | 1042 | A    |
| 47  | 2m    | 1043 | G    |
| 47  | 2m    | 1060 | A    |
| 47  | 2m    | 1061 | U    |
| 47  | 2m    | 1062 | A    |
| 47  | 2m    | 1083 | A    |
| 47  | 2m    | 1085 | C    |
| 47  | 2m    | 1088 | U    |
| 47  | 2m    | 1089 | G    |
| 47  | 2m    | 1110 | G    |
| 47  | 2m    | 1113 | A    |
| 47  | 2m    | 1114 | U    |
| 47  | 2m    | 1115 | U    |
| 47  | 2m    | 1116 | C    |
| 47  | 2m    | 1119 | A    |
| 47  | 2m    | 1131 | G    |
| 47  | 2m    | 1133 | A    |
| 47  | 2m    | 1139 | C    |
| 47  | 2m    | 1150 | A    |
| 47  | 2m    | 1153 | C    |
| 47  | 2m    | 1154 | U    |
| 47  | 2m    | 1157 | G    |
| 47  | 2m    | 1181 | A    |
| 47  | 2m    | 1183 | A    |
| 47  | 2m    | 1195 | A    |
| 47  | 2m    | 1207 | G    |
| 47  | 2m    | 1208 | A    |
| 47  | 2m    | 1215 | C    |
| 47  | 2m    | 1216 | C    |
| 47  | 2m    | 1217 | A    |
| 47  | 2m    | 1221 | G    |
| 47  | 2m    | 1224 | G    |
| 47  | 2m    | 1241 | A    |
| 47  | 2m    | 1242 | U    |
| 47  | 2m    | 1243 | U    |
| 47  | 2m    | 1251 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | 2m    | 1253 | A    |
| 47  | 2m    | 1256 | G    |
| 47  | 2m    | 1257 | G    |
| 47  | 2m    | 1260 | A    |
| 47  | 2m    | 1261 | C    |
| 47  | 2m    | 1262 | C    |
| 47  | 2m    | 1263 | U    |
| 47  | 2m    | 1265 | A    |
| 47  | 2m    | 1273 | C    |
| 47  | 2m    | 1274 | G    |
| 47  | 2m    | 1275 | G    |
| 47  | 2m    | 1280 | G    |
| 47  | 2m    | 1281 | G    |
| 47  | 2m    | 1282 | A    |
| 47  | 2m    | 1283 | C    |
| 47  | 2m    | 1284 | A    |
| 47  | 2m    | 1285 | G    |
| 47  | 2m    | 1286 | G    |
| 47  | 2m    | 1288 | U    |
| 47  | 2m    | 1289 | U    |
| 47  | 2m    | 1290 | G    |
| 47  | 2m    | 1291 | A    |
| 47  | 2m    | 1293 | A    |
| 47  | 2m    | 1294 | G    |
| 47  | 2m    | 1297 | U    |
| 47  | 2m    | 1299 | A    |
| 47  | 2m    | 1300 | U    |
| 47  | 2m    | 1301 | A    |
| 47  | 2m    | 1302 | G    |
| 47  | 2m    | 1303 | C    |
| 47  | 2m    | 1304 | U    |
| 47  | 2m    | 1306 | U    |
| 47  | 2m    | 1307 | U    |
| 47  | 2m    | 1314 | U    |
| 47  | 2m    | 1315 | U    |
| 47  | 2m    | 1316 | C    |
| 47  | 2m    | 1318 | G    |
| 47  | 2m    | 1321 | G    |
| 47  | 2m    | 1326 | U    |
| 47  | 2m    | 1330 | G    |
| 47  | 2m    | 1331 | C    |
| 47  | 2m    | 1332 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | 2m    | 1342 | U    |
| 47  | 2m    | 1371 | U    |
| 47  | 2m    | 1372 | U    |
| 47  | 2m    | 1373 | C    |
| 47  | 2m    | 1375 | G    |
| 47  | 2m    | 1378 | A    |
| 47  | 2m    | 1396 | A    |
| 47  | 2m    | 1397 | U    |
| 47  | 2m    | 1401 | A    |
| 47  | 2m    | 1402 | A    |
| 47  | 2m    | 1403 | C    |
| 47  | 2m    | 1404 | U    |
| 47  | 2m    | 1405 | A    |
| 47  | 2m    | 1407 | U    |
| 47  | 2m    | 1412 | C    |
| 47  | 2m    | 1413 | G    |
| 47  | 2m    | 1414 | A    |
| 47  | 2m    | 1415 | C    |
| 47  | 2m    | 1416 | C    |
| 47  | 2m    | 1417 | C    |
| 47  | 2m    | 1418 | C    |
| 47  | 2m    | 1419 | C    |
| 47  | 2m    | 1420 | G    |
| 47  | 2m    | 1422 | G    |
| 47  | 2m    | 1426 | U    |
| 47  | 2m    | 1427 | C    |
| 47  | 2m    | 1428 | G    |
| 47  | 2m    | 1431 | G    |
| 47  | 2m    | 1436 | C    |
| 47  | 2m    | 1438 | A    |
| 47  | 2m    | 1439 | A    |
| 47  | 2m    | 1440 | C    |
| 47  | 2m    | 1442 | U    |
| 47  | 2m    | 1444 | U    |
| 47  | 2m    | 1449 | G    |
| 47  | 2m    | 1450 | G    |
| 47  | 2m    | 1454 | A    |
| 47  | 2m    | 1462 | U    |
| 47  | 2m    | 1463 | U    |
| 47  | 2m    | 1465 | A    |
| 47  | 2m    | 1473 | G    |
| 47  | 2m    | 1475 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | 2m    | 1476 | A    |
| 47  | 2m    | 1477 | U    |
| 47  | 2m    | 1487 | A    |
| 47  | 2m    | 1489 | A    |
| 47  | 2m    | 1490 | G    |
| 47  | 2m    | 1494 | U    |
| 47  | 2m    | 1498 | A    |
| 47  | 2m    | 1505 | U    |
| 47  | 2m    | 1507 | G    |
| 47  | 2m    | 1508 | A    |
| 47  | 2m    | 1510 | G    |
| 47  | 2m    | 1512 | C    |
| 47  | 2m    | 1515 | G    |
| 47  | 2m    | 1517 | G    |
| 47  | 2m    | 1520 | G    |
| 47  | 2m    | 1521 | C    |
| 47  | 2m    | 1522 | A    |
| 47  | 2m    | 1523 | C    |
| 47  | 2m    | 1524 | G    |
| 47  | 2m    | 1526 | G    |
| 47  | 2m    | 1527 | C    |
| 47  | 2m    | 1533 | A    |
| 47  | 2m    | 1539 | U    |
| 47  | 2m    | 1543 | U    |
| 47  | 2m    | 1544 | C    |
| 47  | 2m    | 1548 | G    |
| 47  | 2m    | 1552 | G    |
| 47  | 2m    | 1553 | C    |
| 47  | 2m    | 1554 | C    |
| 47  | 2m    | 1567 | G    |
| 47  | 2m    | 1570 | G    |
| 47  | 2m    | 1575 | G    |
| 47  | 2m    | 1580 | A    |
| 47  | 2m    | 1585 | U    |
| 47  | 2m    | 1586 | U    |
| 47  | 2m    | 1587 | G    |
| 47  | 2m    | 1588 | A    |
| 47  | 2m    | 1589 | A    |
| 47  | 2m    | 1591 | C    |
| 47  | 2m    | 1594 | A    |
| 47  | 2m    | 1598 | G    |
| 47  | 2m    | 1602 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | 2m    | 1604 | G    |
| 47  | 2m    | 1621 | U    |
| 47  | 2m    | 1623 | A    |
| 47  | 2m    | 1624 | U    |
| 47  | 2m    | 1626 | C    |
| 47  | 2m    | 1627 | C    |
| 47  | 2m    | 1628 | C    |
| 47  | 2m    | 1632 | G    |
| 47  | 2m    | 1634 | A    |
| 47  | 2m    | 1637 | A    |
| 47  | 2m    | 1639 | G    |
| 47  | 2m    | 1644 | C    |
| 47  | 2m    | 1648 | G    |
| 47  | 2m    | 1654 | G    |
| 47  | 2m    | 1664 | A    |
| 47  | 2m    | 1665 | G    |
| 47  | 2m    | 1666 | C    |
| 47  | 2m    | 1672 | U    |
| 47  | 2m    | 1680 | G    |
| 47  | 2m    | 1694 | U    |
| 47  | 2m    | 1695 | A    |
| 47  | 2m    | 1699 | A    |
| 47  | 2m    | 1719 | A    |
| 47  | 2m    | 1721 | U    |
| 47  | 2m    | 1722 | G    |
| 47  | 2m    | 1742 | C    |
| 47  | 2m    | 1743 | G    |
| 47  | 2m    | 1744 | G    |
| 47  | 2m    | 1745 | A    |
| 47  | 2m    | 1746 | U    |
| 47  | 2m    | 1753 | C    |
| 47  | 2m    | 1755 | C    |
| 47  | 2m    | 1756 | C    |
| 47  | 2m    | 1758 | G    |
| 47  | 2m    | 1759 | G    |
| 47  | 2m    | 1761 | U    |
| 47  | 2m    | 1773 | C    |
| 47  | 2m    | 1779 | G    |
| 47  | 2m    | 1780 | G    |
| 47  | 2m    | 1781 | A    |
| 47  | 2m    | 1782 | G    |
| 47  | 2m    | 1783 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 47  | 2m    | 1786 | U    |
| 47  | 2m    | 1813 | A    |
| 47  | 2m    | 1815 | A    |
| 47  | 2m    | 1819 | A    |
| 47  | 2m    | 1821 | U    |
| 47  | 2m    | 1829 | G    |
| 47  | 2m    | 1838 | U    |
| 47  | 2m    | 1849 | G    |
| 47  | 2m    | 1850 | A    |
| 47  | 2m    | 1851 | A    |
| 47  | 2m    | 1852 | C    |
| 47  | 2m    | 1860 | A    |
| 47  | 2m    | 1861 | G    |
| 47  | 2m    | 1862 | G    |
| 47  | 2m    | 1863 | A    |
| 47  | 2m    | 1864 | U    |
| 47  | 2m    | 1865 | C    |
| 47  | 2m    | 1869 | A    |

All (58) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1    | C    |
| 1   | 1A    | 66   | A    |
| 1   | 1A    | 179  | G    |
| 1   | 1A    | 264  | C    |
| 1   | 1A    | 385  | A    |
| 1   | 1A    | 406  | C    |
| 1   | 1A    | 408  | A    |
| 1   | 1A    | 417  | G    |
| 1   | 1A    | 485  | C    |
| 1   | 1A    | 499  | G    |
| 1   | 1A    | 504  | G    |
| 1   | 1A    | 914  | U    |
| 1   | 1A    | 1048 | G    |
| 1   | 1A    | 1173 | G    |
| 1   | 1A    | 1180 | C    |
| 1   | 1A    | 1197 | C    |
| 1   | 1A    | 1220 | G    |
| 1   | 1A    | 1590 | C    |
| 1   | 1A    | 1633 | G    |
| 1   | 1A    | 2017 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2019 | C    |
| 1   | 1A    | 2033 | A    |
| 1   | 1A    | 2112 | G    |
| 1   | 1A    | 2299 | G    |
| 1   | 1A    | 2389 | A    |
| 1   | 1A    | 2503 | G    |
| 1   | 1A    | 2639 | U    |
| 1   | 1A    | 2675 | G    |
| 1   | 1A    | 2695 | A    |
| 1   | 1A    | 2710 | C    |
| 1   | 1A    | 2760 | G    |
| 1   | 1A    | 2775 | C    |
| 1   | 1A    | 3710 | G    |
| 1   | 1A    | 3773 | U    |
| 1   | 1A    | 3810 | C    |
| 1   | 1A    | 3888 | G    |
| 1   | 1A    | 3922 | G    |
| 1   | 1A    | 4060 | U    |
| 1   | 1A    | 4065 | G    |
| 1   | 1A    | 4098 | A    |
| 1   | 1A    | 4099 | G    |
| 1   | 1A    | 4108 | G    |
| 1   | 1A    | 4109 | G    |
| 1   | 1A    | 4110 | C    |
| 1   | 1A    | 4348 | A    |
| 1   | 1A    | 4452 | U    |
| 1   | 1A    | 4599 | A    |
| 1   | 1A    | 4600 | G    |
| 1   | 1A    | 4699 | U    |
| 1   | 1A    | 4731 | G    |
| 1   | 1A    | 4774 | C    |
| 1   | 1A    | 4860 | G    |
| 1   | 1A    | 4896 | G    |
| 1   | 1A    | 4913 | G    |
| 2   | 1B    | 33   | U    |
| 2   | 1B    | 109  | U    |
| 3   | 1C    | 16   | G    |
| 3   | 1C    | 87   | G    |

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 41  | MLZ  | 2g    | 98  | 41   | 8,9,10       | 0.88 | 1 (12%)     | 4,9,11      | 0.57 | 0           |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 41  | MLZ  | 2g    | 98  | 41   | -       | 2/7/8/10 | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 41  | 2g    | 98  | MLZ  | O-C   | 2.04 | 1.27        | 1.20     |

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 41  | 2g    | 98  | MLZ  | CD-CE-NZ-CM |
| 41  | 2g    | 98  | MLZ  | C-CA-CB-CG  |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 425 ligands modelled in this entry, 401 are monoatomic - leaving 24 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 |
| 81  | 84D  | 2m    | 1902 | -    | 32,33,33     | 1.55 | 7 (21%)  | 40,48,48    | 1.13 | 4 (10%)  |
| 81  | 84D  | 1A    | 5114 | -    | 32,33,33     | 1.56 | 7 (21%)  | 40,48,48    | 1.15 | 5 (12%)  |
| 81  | 84D  | 1A    | 5118 | -    | 32,33,33     | 1.56 | 7 (21%)  | 40,48,48    | 1.00 | 3 (7%)   |
| 81  | 84D  | 1A    | 5119 | -    | 32,33,33     | 1.54 | 6 (18%)  | 40,48,48    | 1.11 | 3 (7%)   |
| 81  | 84D  | 1A    | 5104 | -    | 32,33,33     | 1.61 | 9 (28%)  | 40,48,48    | 1.81 | 4 (10%)  |
| 81  | 84D  | 1A    | 5102 | -    | 32,33,33     | 1.57 | 7 (21%)  | 40,48,48    | 1.28 | 4 (10%)  |
| 81  | 84D  | 1A    | 5117 | -    | 32,33,33     | 1.57 | 7 (21%)  | 40,48,48    | 1.21 | 4 (10%)  |
| 81  | 84D  | 1A    | 5112 | -    | 32,33,33     | 1.60 | 7 (21%)  | 40,48,48    | 1.32 | 5 (12%)  |
| 81  | 84D  | 2m    | 1901 | -    | 32,33,33     | 1.54 | 6 (18%)  | 40,48,48    | 1.13 | 7 (17%)  |
| 81  | 84D  | 1A    | 5110 | -    | 32,33,33     | 1.55 | 7 (21%)  | 40,48,48    | 1.16 | 4 (10%)  |
| 81  | 84D  | 2m    | 1903 | -    | 32,33,33     | 1.56 | 6 (18%)  | 40,48,48    | 1.13 | 6 (15%)  |
| 81  | 84D  | 1A    | 5116 | -    | 32,33,33     | 1.53 | 6 (18%)  | 40,48,48    | 1.07 | 2 (5%)   |
| 81  | 84D  | 1A    | 5106 | -    | 32,33,33     | 1.55 | 7 (21%)  | 40,48,48    | 1.15 | 5 (12%)  |
| 81  | 84D  | 1A    | 5109 | -    | 32,33,33     | 1.68 | 7 (21%)  | 40,48,48    | 1.83 | 8 (20%)  |
| 81  | 84D  | 1A    | 5121 | -    | 32,33,33     | 1.54 | 7 (21%)  | 40,48,48    | 1.04 | 3 (7%)   |
| 81  | 84D  | 1A    | 5120 | -    | 32,33,33     | 1.54 | 6 (18%)  | 40,48,48    | 1.12 | 3 (7%)   |
| 81  | 84D  | 1A    | 5108 | -    | 32,33,33     | 1.55 | 6 (18%)  | 40,48,48    | 1.20 | 3 (7%)   |
| 81  | 84D  | 1A    | 5107 | -    | 32,33,33     | 1.59 | 7 (21%)  | 40,48,48    | 1.14 | 4 (10%)  |
| 81  | 84D  | 1A    | 5111 | -    | 32,33,33     | 1.56 | 7 (21%)  | 40,48,48    | 1.00 | 2 (5%)   |
| 81  | 84D  | 1A    | 5105 | -    | 32,33,33     | 1.61 | 7 (21%)  | 40,48,48    | 1.38 | 6 (15%)  |
| 81  | 84D  | 1A    | 5115 | -    | 32,33,33     | 1.57 | 7 (21%)  | 40,48,48    | 1.08 | 4 (10%)  |
| 81  | 84D  | 1A    | 5113 | -    | 32,33,33     | 1.57 | 7 (21%)  | 40,48,48    | 1.25 | 6 (15%)  |
| 81  | 84D  | 1A    | 5101 | -    | 32,33,33     | 1.56 | 7 (21%)  | 40,48,48    | 1.06 | 3 (7%)   |
| 81  | 84D  | 1A    | 5103 | -    | 32,33,33     | 1.52 | 6 (18%)  | 40,48,48    | 1.21 | 4 (10%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 81  | 84D  | 2m    | 1902 | -    | -       | 3/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5114 | -    | -       | 3/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5118 | -    | -       | 6/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5119 | -    | -       | 3/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5104 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5102 | -    | -       | 2/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5117 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5112 | -    | -       | 2/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 2m    | 1901 | -    | -       | 3/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5110 | -    | -       | 3/12/65/65 | 1/3/3/3 |
| 81  | 84D  | 2m    | 1903 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5116 | -    | -       | 5/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5106 | -    | -       | 7/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5109 | -    | -       | 3/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5121 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5120 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5108 | -    | -       | 6/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5107 | -    | -       | 2/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5111 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5105 | -    | -       | 3/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5115 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5113 | -    | -       | 4/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5101 | -    | -       | 5/12/65/65 | 0/3/3/3 |
| 81  | 84D  | 1A    | 5103 | -    | -       | 3/12/65/65 | 0/3/3/3 |

All (163) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | 1A    | 5109 | 84D  | C15-C14 | -5.13 | 1.47        | 1.53     |
| 81  | 1A    | 5112 | 84D  | C15-C14 | -4.86 | 1.47        | 1.53     |
| 81  | 1A    | 5102 | 84D  | C15-C14 | -4.70 | 1.47        | 1.53     |
| 81  | 1A    | 5104 | 84D  | C15-C14 | -4.62 | 1.47        | 1.53     |
| 81  | 1A    | 5113 | 84D  | C15-C14 | -4.58 | 1.47        | 1.53     |
| 81  | 1A    | 5106 | 84D  | C15-C14 | -4.57 | 1.47        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | 1A    | 5107 | 84D  | C15-C14 | -4.53 | 1.47        | 1.53     |
| 81  | 1A    | 5118 | 84D  | C15-C14 | -4.53 | 1.47        | 1.53     |
| 81  | 1A    | 5111 | 84D  | C15-C14 | -4.50 | 1.47        | 1.53     |
| 81  | 1A    | 5115 | 84D  | C15-C14 | -4.47 | 1.47        | 1.53     |
| 81  | 1A    | 5101 | 84D  | C15-C14 | -4.45 | 1.48        | 1.53     |
| 81  | 1A    | 5110 | 84D  | C15-C14 | -4.44 | 1.48        | 1.53     |
| 81  | 1A    | 5117 | 84D  | C15-C14 | -4.42 | 1.48        | 1.53     |
| 81  | 1A    | 5120 | 84D  | C15-C14 | -4.41 | 1.48        | 1.53     |
| 81  | 1A    | 5114 | 84D  | C15-C14 | -4.34 | 1.48        | 1.53     |
| 81  | 2m    | 1902 | 84D  | C15-C14 | -4.31 | 1.48        | 1.53     |
| 81  | 1A    | 5103 | 84D  | C15-C14 | -4.30 | 1.48        | 1.53     |
| 81  | 2m    | 1903 | 84D  | C15-C14 | -4.30 | 1.48        | 1.53     |
| 81  | 1A    | 5105 | 84D  | C15-C14 | -4.30 | 1.48        | 1.53     |
| 81  | 1A    | 5119 | 84D  | C15-C14 | -4.29 | 1.48        | 1.53     |
| 81  | 1A    | 5121 | 84D  | C15-C14 | -4.29 | 1.48        | 1.53     |
| 81  | 1A    | 5108 | 84D  | C15-C14 | -4.26 | 1.48        | 1.53     |
| 81  | 1A    | 5116 | 84D  | C15-C14 | -4.25 | 1.48        | 1.53     |
| 81  | 2m    | 1901 | 84D  | C15-C14 | -4.24 | 1.48        | 1.53     |
| 81  | 1A    | 5105 | 84D  | C13-C14 | -3.91 | 1.48        | 1.53     |
| 81  | 1A    | 5109 | 84D  | C13-C14 | -3.64 | 1.49        | 1.53     |
| 81  | 1A    | 5110 | 84D  | C13-C14 | -3.56 | 1.49        | 1.53     |
| 81  | 1A    | 5115 | 84D  | C13-C14 | -3.51 | 1.49        | 1.53     |
| 81  | 1A    | 5117 | 84D  | C13-C14 | -3.50 | 1.49        | 1.53     |
| 81  | 1A    | 5107 | 84D  | C13-C14 | -3.50 | 1.49        | 1.53     |
| 81  | 2m    | 1903 | 84D  | C13-C14 | -3.47 | 1.49        | 1.53     |
| 81  | 1A    | 5101 | 84D  | C13-C14 | -3.46 | 1.49        | 1.53     |
| 81  | 2m    | 1901 | 84D  | C13-C14 | -3.44 | 1.49        | 1.53     |
| 81  | 1A    | 5114 | 84D  | C13-C14 | -3.43 | 1.49        | 1.53     |
| 81  | 1A    | 5104 | 84D  | C13-C14 | -3.39 | 1.49        | 1.53     |
| 81  | 1A    | 5111 | 84D  | C13-C14 | -3.39 | 1.49        | 1.53     |
| 81  | 1A    | 5116 | 84D  | C13-C14 | -3.37 | 1.49        | 1.53     |
| 81  | 1A    | 5118 | 84D  | C13-C14 | -3.36 | 1.49        | 1.53     |
| 81  | 1A    | 5106 | 84D  | C13-C14 | -3.36 | 1.49        | 1.53     |
| 81  | 1A    | 5108 | 84D  | C13-C14 | -3.33 | 1.49        | 1.53     |
| 81  | 2m    | 1902 | 84D  | C13-C14 | -3.32 | 1.49        | 1.53     |
| 81  | 1A    | 5121 | 84D  | C13-C14 | -3.32 | 1.49        | 1.53     |
| 81  | 1A    | 5119 | 84D  | C13-C14 | -3.26 | 1.49        | 1.53     |
| 81  | 1A    | 5112 | 84D  | C13-C14 | -3.26 | 1.49        | 1.53     |
| 81  | 1A    | 5113 | 84D  | C14-N1  | 3.22  | 1.52        | 1.47     |
| 81  | 1A    | 5120 | 84D  | C13-C14 | -3.22 | 1.49        | 1.53     |
| 81  | 1A    | 5103 | 84D  | C14-N1  | 3.22  | 1.52        | 1.47     |
| 81  | 1A    | 5121 | 84D  | C14-N1  | 3.20  | 1.52        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | 2m    | 1902 | 84D  | C14-N1  | 3.19  | 1.52        | 1.47     |
| 81  | 1A    | 5114 | 84D  | C14-N1  | 3.19  | 1.52        | 1.47     |
| 81  | 2m    | 1903 | 84D  | C14-N1  | 3.18  | 1.52        | 1.47     |
| 81  | 1A    | 5112 | 84D  | C14-N1  | 3.18  | 1.52        | 1.47     |
| 81  | 1A    | 5116 | 84D  | C14-N1  | 3.18  | 1.52        | 1.47     |
| 81  | 1A    | 5106 | 84D  | C14-N1  | 3.17  | 1.52        | 1.47     |
| 81  | 1A    | 5105 | 84D  | C14-N1  | 3.17  | 1.52        | 1.47     |
| 81  | 1A    | 5118 | 84D  | C14-N1  | 3.17  | 1.52        | 1.47     |
| 81  | 2m    | 1901 | 84D  | C14-N1  | 3.16  | 1.52        | 1.47     |
| 81  | 1A    | 5120 | 84D  | C14-N1  | 3.15  | 1.52        | 1.47     |
| 81  | 1A    | 5110 | 84D  | C14-N1  | 3.15  | 1.52        | 1.47     |
| 81  | 1A    | 5115 | 84D  | C14-N1  | 3.15  | 1.52        | 1.47     |
| 81  | 1A    | 5119 | 84D  | C14-N1  | 3.14  | 1.52        | 1.47     |
| 81  | 1A    | 5102 | 84D  | C13-C14 | -3.14 | 1.49        | 1.53     |
| 81  | 1A    | 5102 | 84D  | C14-N1  | 3.14  | 1.52        | 1.47     |
| 81  | 1A    | 5117 | 84D  | C14-N1  | 3.13  | 1.52        | 1.47     |
| 81  | 1A    | 5113 | 84D  | C13-C14 | -3.13 | 1.49        | 1.53     |
| 81  | 1A    | 5101 | 84D  | C14-N1  | 3.13  | 1.52        | 1.47     |
| 81  | 1A    | 5108 | 84D  | C14-N1  | 3.12  | 1.52        | 1.47     |
| 81  | 1A    | 5111 | 84D  | C14-N1  | 3.11  | 1.52        | 1.47     |
| 81  | 1A    | 5104 | 84D  | C14-N1  | 3.11  | 1.52        | 1.47     |
| 81  | 1A    | 5109 | 84D  | C14-N1  | 3.11  | 1.52        | 1.47     |
| 81  | 1A    | 5103 | 84D  | C13-C14 | -3.10 | 1.49        | 1.53     |
| 81  | 1A    | 5107 | 84D  | C14-N1  | 3.10  | 1.52        | 1.47     |
| 81  | 1A    | 5112 | 84D  | O-C3    | 2.72  | 1.48        | 1.41     |
| 81  | 1A    | 5113 | 84D  | O-C3    | 2.72  | 1.48        | 1.41     |
| 81  | 1A    | 5109 | 84D  | O-C3    | 2.71  | 1.48        | 1.41     |
| 81  | 1A    | 5107 | 84D  | O-C3    | 2.68  | 1.48        | 1.41     |
| 81  | 1A    | 5108 | 84D  | O-C3    | 2.67  | 1.48        | 1.41     |
| 81  | 2m    | 1903 | 84D  | O-C3    | 2.63  | 1.48        | 1.41     |
| 81  | 1A    | 5119 | 84D  | O-C3    | 2.62  | 1.48        | 1.41     |
| 81  | 1A    | 5102 | 84D  | O-C3    | 2.61  | 1.48        | 1.41     |
| 81  | 1A    | 5114 | 84D  | O-C3    | 2.60  | 1.48        | 1.41     |
| 81  | 1A    | 5105 | 84D  | O-C3    | 2.59  | 1.48        | 1.41     |
| 81  | 2m    | 1901 | 84D  | O-C3    | 2.59  | 1.48        | 1.41     |
| 81  | 1A    | 5116 | 84D  | O-C3    | 2.58  | 1.48        | 1.41     |
| 81  | 1A    | 5105 | 84D  | O4-C16  | 2.54  | 1.50        | 1.44     |
| 81  | 1A    | 5120 | 84D  | O-C3    | 2.52  | 1.48        | 1.41     |
| 81  | 1A    | 5101 | 84D  | O-C3    | 2.52  | 1.48        | 1.41     |
| 81  | 1A    | 5115 | 84D  | O-C3    | 2.52  | 1.48        | 1.41     |
| 81  | 1A    | 5118 | 84D  | O-C3    | 2.51  | 1.48        | 1.41     |
| 81  | 1A    | 5104 | 84D  | O-C3    | 2.49  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | 2m    | 1902 | 84D  | O-C3   | 2.49  | 1.48        | 1.41     |
| 81  | 1A    | 5110 | 84D  | O-C3   | 2.47  | 1.48        | 1.41     |
| 81  | 1A    | 5109 | 84D  | O4-C12 | 2.47  | 1.48        | 1.41     |
| 81  | 1A    | 5111 | 84D  | O-C3   | 2.46  | 1.48        | 1.41     |
| 81  | 1A    | 5103 | 84D  | O-C3   | 2.46  | 1.48        | 1.41     |
| 81  | 1A    | 5117 | 84D  | O-C3   | 2.42  | 1.48        | 1.41     |
| 81  | 1A    | 5121 | 84D  | O-C3   | 2.42  | 1.48        | 1.41     |
| 81  | 1A    | 5106 | 84D  | O-C3   | 2.41  | 1.48        | 1.41     |
| 81  | 1A    | 5112 | 84D  | O4-C12 | 2.37  | 1.47        | 1.41     |
| 81  | 1A    | 5109 | 84D  | C-C1   | -2.35 | 1.47        | 1.52     |
| 81  | 1A    | 5107 | 84D  | O4-C16 | 2.34  | 1.50        | 1.44     |
| 81  | 2m    | 1903 | 84D  | O4-C16 | 2.31  | 1.50        | 1.44     |
| 81  | 1A    | 5117 | 84D  | O4-C16 | 2.29  | 1.50        | 1.44     |
| 81  | 1A    | 5111 | 84D  | O4-C16 | 2.28  | 1.50        | 1.44     |
| 81  | 1A    | 5104 | 84D  | O-C4   | 2.28  | 1.47        | 1.44     |
| 81  | 1A    | 5114 | 84D  | O4-C16 | 2.28  | 1.49        | 1.44     |
| 81  | 1A    | 5104 | 84D  | O4-C16 | 2.28  | 1.49        | 1.44     |
| 81  | 1A    | 5113 | 84D  | O4-C12 | 2.25  | 1.47        | 1.41     |
| 81  | 2m    | 1902 | 84D  | O4-C16 | 2.25  | 1.49        | 1.44     |
| 81  | 1A    | 5113 | 84D  | C-C1   | -2.24 | 1.47        | 1.52     |
| 81  | 1A    | 5115 | 84D  | O4-C16 | 2.24  | 1.49        | 1.44     |
| 81  | 1A    | 5112 | 84D  | C-C1   | -2.24 | 1.47        | 1.52     |
| 81  | 1A    | 5121 | 84D  | O4-C16 | 2.23  | 1.49        | 1.44     |
| 81  | 2m    | 1901 | 84D  | O4-C16 | 2.23  | 1.49        | 1.44     |
| 81  | 1A    | 5108 | 84D  | O4-C16 | 2.23  | 1.49        | 1.44     |
| 81  | 1A    | 5109 | 84D  | O4-C16 | 2.22  | 1.49        | 1.44     |
| 81  | 1A    | 5102 | 84D  | O4-C12 | 2.22  | 1.47        | 1.41     |
| 81  | 1A    | 5114 | 84D  | C-C1   | -2.22 | 1.47        | 1.52     |
| 81  | 1A    | 5101 | 84D  | O4-C16 | 2.21  | 1.49        | 1.44     |
| 81  | 1A    | 5110 | 84D  | O4-C16 | 2.21  | 1.49        | 1.44     |
| 81  | 1A    | 5104 | 84D  | C-C1   | -2.21 | 1.47        | 1.52     |
| 81  | 1A    | 5120 | 84D  | O4-C16 | 2.20  | 1.49        | 1.44     |
| 81  | 1A    | 5107 | 84D  | C-C1   | -2.20 | 1.47        | 1.52     |
| 81  | 1A    | 5108 | 84D  | C-C1   | -2.19 | 1.47        | 1.52     |
| 81  | 1A    | 5116 | 84D  | O4-C16 | 2.19  | 1.49        | 1.44     |
| 81  | 1A    | 5112 | 84D  | O4-C16 | 2.19  | 1.49        | 1.44     |
| 81  | 1A    | 5102 | 84D  | C-C1   | -2.19 | 1.47        | 1.52     |
| 81  | 1A    | 5106 | 84D  | O4-C12 | 2.17  | 1.47        | 1.41     |
| 81  | 1A    | 5119 | 84D  | C-C1   | -2.16 | 1.47        | 1.52     |
| 81  | 1A    | 5113 | 84D  | O4-C16 | 2.16  | 1.49        | 1.44     |
| 81  | 1A    | 5105 | 84D  | C-C1   | -2.16 | 1.47        | 1.52     |
| 81  | 1A    | 5118 | 84D  | O4-C12 | 2.15  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 81  | 1A    | 5119 | 84D  | O4-C16 | 2.15  | 1.49        | 1.44     |
| 81  | 2m    | 1903 | 84D  | C-C1   | -2.15 | 1.47        | 1.52     |
| 81  | 1A    | 5105 | 84D  | O4-C12 | 2.15  | 1.47        | 1.41     |
| 81  | 1A    | 5118 | 84D  | O4-C16 | 2.15  | 1.49        | 1.44     |
| 81  | 1A    | 5116 | 84D  | C-C1   | -2.14 | 1.47        | 1.52     |
| 81  | 1A    | 5120 | 84D  | C-C1   | -2.14 | 1.47        | 1.52     |
| 81  | 1A    | 5104 | 84D  | O4-C12 | 2.13  | 1.47        | 1.41     |
| 81  | 2m    | 1901 | 84D  | C-C1   | -2.12 | 1.47        | 1.52     |
| 81  | 1A    | 5115 | 84D  | C-C1   | -2.12 | 1.47        | 1.52     |
| 81  | 1A    | 5107 | 84D  | O4-C12 | 2.11  | 1.47        | 1.41     |
| 81  | 1A    | 5118 | 84D  | C-C1   | -2.11 | 1.47        | 1.52     |
| 81  | 1A    | 5103 | 84D  | O4-C16 | 2.10  | 1.49        | 1.44     |
| 81  | 1A    | 5104 | 84D  | C1-C2  | -2.09 | 1.47        | 1.53     |
| 81  | 1A    | 5106 | 84D  | C-C1   | -2.09 | 1.47        | 1.52     |
| 81  | 1A    | 5111 | 84D  | O4-C12 | 2.09  | 1.47        | 1.41     |
| 81  | 1A    | 5106 | 84D  | O4-C16 | 2.08  | 1.49        | 1.44     |
| 81  | 1A    | 5101 | 84D  | O4-C12 | 2.08  | 1.47        | 1.41     |
| 81  | 1A    | 5102 | 84D  | O4-C16 | 2.08  | 1.49        | 1.44     |
| 81  | 1A    | 5103 | 84D  | C-C1   | -2.08 | 1.47        | 1.52     |
| 81  | 1A    | 5115 | 84D  | O4-C12 | 2.07  | 1.47        | 1.41     |
| 81  | 1A    | 5101 | 84D  | C-C1   | -2.07 | 1.47        | 1.52     |
| 81  | 1A    | 5117 | 84D  | C-C1   | -2.06 | 1.47        | 1.52     |
| 81  | 2m    | 1902 | 84D  | C-C1   | -2.06 | 1.47        | 1.52     |
| 81  | 1A    | 5111 | 84D  | C-C1   | -2.05 | 1.47        | 1.52     |
| 81  | 1A    | 5117 | 84D  | O4-C12 | 2.04  | 1.47        | 1.41     |
| 81  | 1A    | 5110 | 84D  | C-C1   | -2.03 | 1.48        | 1.52     |
| 81  | 2m    | 1902 | 84D  | O4-C12 | 2.03  | 1.47        | 1.41     |
| 81  | 1A    | 5121 | 84D  | C-C1   | -2.02 | 1.48        | 1.52     |
| 81  | 1A    | 5110 | 84D  | O4-C12 | 2.01  | 1.47        | 1.41     |
| 81  | 1A    | 5121 | 84D  | O4-C12 | 2.00  | 1.47        | 1.41     |
| 81  | 1A    | 5114 | 84D  | O4-C12 | 2.00  | 1.47        | 1.41     |

All (102) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 81  | 1A    | 5104 | 84D  | O-C4-C      | 8.07 | 118.40      | 109.91   |
| 81  | 1A    | 5109 | 84D  | C3-O-C4     | 4.66 | 118.30      | 113.13   |
| 81  | 1A    | 5104 | 84D  | C3-O-C4     | 4.14 | 117.72      | 113.13   |
| 81  | 1A    | 5109 | 84D  | O4-C12-C13  | 4.08 | 118.76      | 110.37   |
| 81  | 1A    | 5105 | 84D  | C16-C15-C14 | 4.06 | 115.16      | 110.67   |
| 81  | 1A    | 5109 | 84D  | C12-C13-C14 | 3.85 | 115.58      | 110.40   |
| 81  | 1A    | 5109 | 84D  | O-C4-C      | 3.68 | 113.78      | 109.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | 1A    | 5102 | 84D  | C12-C13-C14 | 3.66  | 115.31      | 110.40   |
| 81  | 1A    | 5112 | 84D  | C12-C13-C14 | 3.53  | 115.14      | 110.40   |
| 81  | 1A    | 5109 | 84D  | O-C3-C2     | 3.45  | 117.84      | 110.26   |
| 81  | 1A    | 5113 | 84D  | C12-C13-C14 | 3.40  | 114.97      | 110.40   |
| 81  | 1A    | 5103 | 84D  | O-C4-C      | 3.36  | 113.44      | 109.91   |
| 81  | 1A    | 5119 | 84D  | O-C4-C      | 3.34  | 113.42      | 109.91   |
| 81  | 1A    | 5105 | 84D  | O4-C16-C15  | 3.29  | 115.63      | 109.70   |
| 81  | 1A    | 5112 | 84D  | C3-O1-C6    | -3.26 | 110.25      | 117.98   |
| 81  | 1A    | 5102 | 84D  | C3-O1-C6    | -3.24 | 110.30      | 117.98   |
| 81  | 1A    | 5109 | 84D  | C12-O3-C10  | -3.18 | 110.44      | 117.98   |
| 81  | 1A    | 5103 | 84D  | C3-O1-C6    | -3.15 | 110.51      | 117.98   |
| 81  | 1A    | 5104 | 84D  | C1-C-C4     | 3.15  | 116.02      | 110.96   |
| 81  | 1A    | 5110 | 84D  | O-C4-C      | 3.11  | 113.18      | 109.91   |
| 81  | 1A    | 5104 | 84D  | C-C4-C5     | -3.11 | 106.89      | 112.83   |
| 81  | 1A    | 5106 | 84D  | C12-O3-C10  | -3.09 | 110.65      | 117.98   |
| 81  | 1A    | 5120 | 84D  | O-C4-C      | 3.04  | 113.11      | 109.91   |
| 81  | 1A    | 5118 | 84D  | C3-O1-C6    | -3.03 | 110.79      | 117.98   |
| 81  | 1A    | 5117 | 84D  | C10-C11-C6  | 3.01  | 115.22      | 109.11   |
| 81  | 2m    | 1902 | 84D  | O-C4-C      | 3.00  | 113.06      | 109.91   |
| 81  | 1A    | 5114 | 84D  | C3-O1-C6    | -2.99 | 110.89      | 117.98   |
| 81  | 1A    | 5105 | 84D  | C3-O1-C6    | -2.95 | 110.98      | 117.98   |
| 81  | 1A    | 5107 | 84D  | O-C4-C      | 2.93  | 112.99      | 109.91   |
| 81  | 1A    | 5110 | 84D  | C10-C11-C6  | 2.89  | 114.96      | 109.11   |
| 81  | 1A    | 5117 | 84D  | O-C4-C      | 2.84  | 112.90      | 109.91   |
| 81  | 1A    | 5119 | 84D  | C3-O1-C6    | -2.84 | 111.25      | 117.98   |
| 81  | 1A    | 5112 | 84D  | C12-O3-C10  | -2.81 | 111.33      | 117.98   |
| 81  | 2m    | 1903 | 84D  | C3-O1-C6    | -2.80 | 111.35      | 117.98   |
| 81  | 1A    | 5105 | 84D  | C12-O3-C10  | -2.79 | 111.37      | 117.98   |
| 81  | 1A    | 5108 | 84D  | O-C4-C      | 2.76  | 112.82      | 109.91   |
| 81  | 1A    | 5117 | 84D  | C3-O1-C6    | -2.72 | 111.53      | 117.98   |
| 81  | 1A    | 5102 | 84D  | C12-O3-C10  | -2.72 | 111.54      | 117.98   |
| 81  | 1A    | 5118 | 84D  | O-C4-C      | 2.72  | 112.77      | 109.91   |
| 81  | 1A    | 5101 | 84D  | C3-O1-C6    | -2.71 | 111.56      | 117.98   |
| 81  | 1A    | 5108 | 84D  | C10-C11-C6  | 2.70  | 114.58      | 109.11   |
| 81  | 2m    | 1902 | 84D  | C3-O1-C6    | -2.69 | 111.60      | 117.98   |
| 81  | 1A    | 5107 | 84D  | C3-O1-C6    | -2.64 | 111.72      | 117.98   |
| 81  | 1A    | 5115 | 84D  | C10-C11-C6  | 2.60  | 114.38      | 109.11   |
| 81  | 2m    | 1902 | 84D  | C10-C11-C6  | 2.56  | 114.31      | 109.11   |
| 81  | 2m    | 1903 | 84D  | O-C4-C      | 2.56  | 112.61      | 109.91   |
| 81  | 1A    | 5109 | 84D  | C12-O4-C16  | 2.55  | 118.69      | 113.72   |
| 81  | 1A    | 5116 | 84D  | C3-O1-C6    | -2.53 | 111.97      | 117.98   |
| 81  | 1A    | 5113 | 84D  | C3-O1-C6    | -2.51 | 112.03      | 117.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | 1A    | 5106 | 84D  | C12-C13-C14 | 2.50  | 113.76      | 110.40   |
| 81  | 2m    | 1901 | 84D  | C12-O3-C10  | -2.48 | 112.10      | 117.98   |
| 81  | 1A    | 5101 | 84D  | O-C4-C      | 2.46  | 112.50      | 109.91   |
| 81  | 1A    | 5121 | 84D  | O-C4-C      | 2.45  | 112.48      | 109.91   |
| 81  | 1A    | 5120 | 84D  | C3-O1-C6    | -2.44 | 112.20      | 117.98   |
| 81  | 1A    | 5115 | 84D  | C12-O3-C10  | -2.43 | 112.21      | 117.98   |
| 81  | 1A    | 5109 | 84D  | C10-C11-C6  | 2.42  | 114.01      | 109.11   |
| 81  | 1A    | 5113 | 84D  | C12-O3-C10  | -2.41 | 112.26      | 117.98   |
| 81  | 1A    | 5120 | 84D  | C-C4-C5     | -2.40 | 108.24      | 112.83   |
| 81  | 1A    | 5114 | 84D  | O-C4-C      | 2.39  | 112.43      | 109.91   |
| 81  | 1A    | 5111 | 84D  | C3-O1-C6    | -2.38 | 112.33      | 117.98   |
| 81  | 1A    | 5107 | 84D  | C12-O3-C10  | -2.38 | 112.34      | 117.98   |
| 81  | 1A    | 5112 | 84D  | O4-C12-C13  | 2.37  | 115.24      | 110.37   |
| 81  | 1A    | 5116 | 84D  | O-C4-C      | 2.37  | 112.40      | 109.91   |
| 81  | 1A    | 5106 | 84D  | C3-O1-C6    | -2.36 | 112.39      | 117.98   |
| 81  | 1A    | 5117 | 84D  | C-C4-C5     | -2.33 | 108.38      | 112.83   |
| 81  | 1A    | 5110 | 84D  | C-C4-C5     | -2.29 | 108.46      | 112.83   |
| 81  | 1A    | 5106 | 84D  | C3-O-C4     | -2.29 | 110.60      | 113.13   |
| 81  | 1A    | 5121 | 84D  | C10-C11-C6  | 2.25  | 113.67      | 109.11   |
| 81  | 1A    | 5107 | 84D  | C-C4-C5     | -2.22 | 108.59      | 112.83   |
| 81  | 1A    | 5102 | 84D  | O4-C12-C13  | 2.20  | 114.89      | 110.37   |
| 81  | 1A    | 5119 | 84D  | C-C4-C5     | -2.19 | 108.64      | 112.83   |
| 81  | 1A    | 5108 | 84D  | C-C4-C5     | -2.19 | 108.65      | 112.83   |
| 81  | 2m    | 1903 | 84D  | O4-C16-C15  | 2.18  | 113.63      | 109.70   |
| 81  | 2m    | 1901 | 84D  | C3-O1-C6    | -2.18 | 112.81      | 117.98   |
| 81  | 1A    | 5113 | 84D  | O-C3-C2     | 2.17  | 115.03      | 110.26   |
| 81  | 1A    | 5101 | 84D  | C12-O3-C10  | -2.17 | 112.84      | 117.98   |
| 81  | 1A    | 5110 | 84D  | C12-O3-C10  | -2.17 | 112.84      | 117.98   |
| 81  | 1A    | 5121 | 84D  | C3-O1-C6    | -2.17 | 112.84      | 117.98   |
| 81  | 2m    | 1903 | 84D  | C-C4-C5     | -2.16 | 108.71      | 112.83   |
| 81  | 1A    | 5115 | 84D  | C-C4-C5     | -2.16 | 108.71      | 112.83   |
| 81  | 1A    | 5114 | 84D  | C-C4-C5     | -2.15 | 108.72      | 112.83   |
| 81  | 1A    | 5118 | 84D  | C12-O3-C10  | -2.14 | 112.91      | 117.98   |
| 81  | 2m    | 1901 | 84D  | O-C4-C      | 2.12  | 112.14      | 109.91   |
| 81  | 1A    | 5114 | 84D  | O4-C16-C15  | 2.09  | 113.46      | 109.70   |
| 81  | 2m    | 1903 | 84D  | C12-O3-C10  | -2.09 | 113.03      | 117.98   |
| 81  | 2m    | 1902 | 84D  | C-C4-C5     | -2.08 | 108.85      | 112.83   |
| 81  | 1A    | 5105 | 84D  | O-C4-C      | 2.08  | 112.10      | 109.91   |
| 81  | 1A    | 5111 | 84D  | C12-O3-C10  | -2.08 | 113.06      | 117.98   |
| 81  | 2m    | 1903 | 84D  | C16-C15-C14 | 2.07  | 112.96      | 110.67   |
| 81  | 1A    | 5103 | 84D  | C-C4-C5     | -2.07 | 108.88      | 112.83   |
| 81  | 2m    | 1901 | 84D  | C-C4-C5     | -2.07 | 108.88      | 112.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | 1A    | 5105 | 84D  | C-C4-C5     | -2.06 | 108.89      | 112.83   |
| 81  | 1A    | 5106 | 84D  | C10-C11-C6  | 2.06  | 113.28      | 109.11   |
| 81  | 1A    | 5103 | 84D  | C9-C8-C7    | 2.06  | 114.55      | 111.02   |
| 81  | 1A    | 5112 | 84D  | C-C4-C5     | -2.04 | 108.92      | 112.83   |
| 81  | 1A    | 5113 | 84D  | O4-C12-C13  | 2.03  | 114.54      | 110.37   |
| 81  | 2m    | 1901 | 84D  | C10-C11-C6  | 2.03  | 113.22      | 109.11   |
| 81  | 2m    | 1901 | 84D  | O4-C16-C15  | 2.03  | 113.35      | 109.70   |
| 81  | 2m    | 1901 | 84D  | C16-C15-C14 | 2.02  | 112.91      | 110.67   |
| 81  | 1A    | 5114 | 84D  | C16-C15-C14 | 2.01  | 112.90      | 110.67   |
| 81  | 1A    | 5113 | 84D  | C-C4-C5     | -2.01 | 108.99      | 112.83   |
| 81  | 1A    | 5115 | 84D  | O-C4-C      | 2.00  | 112.02      | 109.91   |

There are no chirality outliers.

All (91) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 81  | 1A    | 5101 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5101 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5104 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5105 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5105 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5106 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5106 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5107 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5108 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5108 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5110 | 84D  | C2-C3-O1-C6 |
| 81  | 1A    | 5111 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5111 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5113 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5113 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5114 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5115 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5116 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5116 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5117 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5117 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5118 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5119 | 84D  | O-C4-C5-N   |
| 81  | 1A    | 5119 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5120 | 84D  | C-C4-C5-N   |
| 81  | 1A    | 5121 | 84D  | O-C4-C5-N   |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 81  | 1A    | 5121 | 84D  | C-C4-C5-N      |
| 81  | 2m    | 1901 | 84D  | O-C4-C5-N      |
| 81  | 2m    | 1902 | 84D  | O-C4-C5-N      |
| 81  | 2m    | 1903 | 84D  | O-C4-C5-N      |
| 81  | 1A    | 5102 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5118 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5112 | 84D  | O4-C16-C17-O5  |
| 81  | 2m    | 1902 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5106 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5120 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5102 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5109 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5114 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5120 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5118 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5109 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5121 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5116 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5114 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5111 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5117 | 84D  | O4-C16-C17-O5  |
| 81  | 2m    | 1902 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5115 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5112 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5117 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5121 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5116 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5111 | 84D  | O4-C16-C17-O5  |
| 81  | 2m    | 1903 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5110 | 84D  | C13-C12-O3-C10 |
| 81  | 1A    | 5110 | 84D  | O4-C12-O3-C10  |
| 81  | 1A    | 5106 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5108 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5118 | 84D  | O4-C12-O3-C10  |
| 81  | 1A    | 5101 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5115 | 84D  | C11-C6-O1-C3   |
| 81  | 2m    | 1903 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5103 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5106 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5108 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5108 | 84D  | C11-C6-O1-C3   |
| 81  | 1A    | 5103 | 84D  | O-C4-C5-N      |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 81  | 1A    | 5109 | 84D  | O-C4-C5-N      |
| 81  | 1A    | 5120 | 84D  | O-C4-C5-N      |
| 81  | 1A    | 5103 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5105 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5115 | 84D  | C7-C6-O1-C3    |
| 81  | 1A    | 5104 | 84D  | C15-C16-C17-O5 |
| 81  | 2m    | 1901 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5107 | 84D  | O4-C16-C17-O5  |
| 81  | 2m    | 1903 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5108 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5104 | 84D  | C11-C6-O1-C3   |
| 81  | 1A    | 5116 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5119 | 84D  | O4-C16-C17-O5  |
| 81  | 1A    | 5104 | 84D  | C2-C3-O1-C6    |
| 81  | 2m    | 1901 | 84D  | C11-C6-O1-C3   |
| 81  | 1A    | 5101 | 84D  | C15-C16-C17-O5 |
| 81  | 1A    | 5118 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5113 | 84D  | O-C3-O1-C6     |
| 81  | 1A    | 5106 | 84D  | C11-C6-O1-C3   |
| 81  | 1A    | 5118 | 84D  | C13-C12-O3-C10 |
| 81  | 1A    | 5113 | 84D  | C11-C6-O1-C3   |
| 81  | 1A    | 5101 | 84D  | C11-C10-O3-C12 |
| 81  | 1A    | 5106 | 84D  | O4-C12-O3-C10  |

All (1) ring outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 81  | 1A    | 5110 | 84D  | C-C1-C2-C3-C4-O |

15 monomers are involved in 26 short contacts:

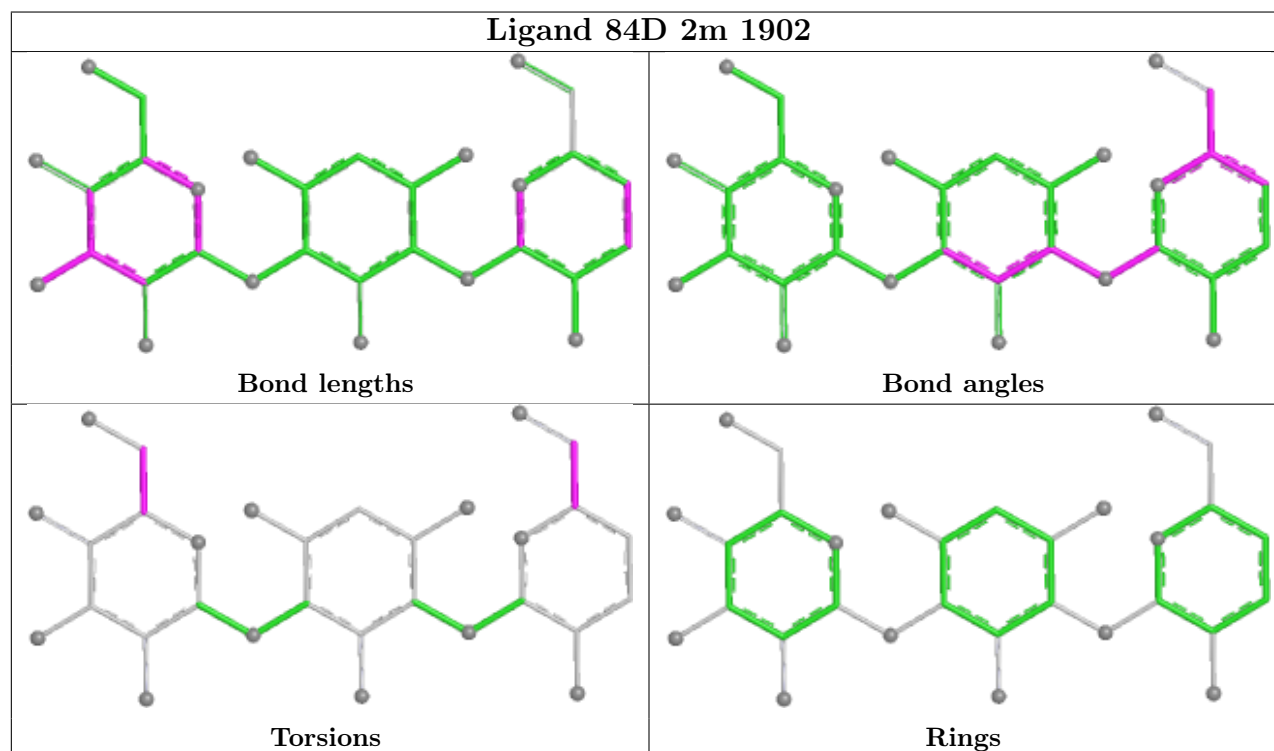
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81  | 2m    | 1902 | 84D  | 2       | 0            |
| 81  | 1A    | 5118 | 84D  | 2       | 0            |
| 81  | 1A    | 5119 | 84D  | 1       | 0            |
| 81  | 1A    | 5104 | 84D  | 3       | 0            |
| 81  | 2m    | 1901 | 84D  | 3       | 0            |
| 81  | 1A    | 5110 | 84D  | 4       | 0            |
| 81  | 2m    | 1903 | 84D  | 1       | 0            |
| 81  | 1A    | 5116 | 84D  | 1       | 0            |
| 81  | 1A    | 5106 | 84D  | 1       | 0            |
| 81  | 1A    | 5109 | 84D  | 1       | 0            |

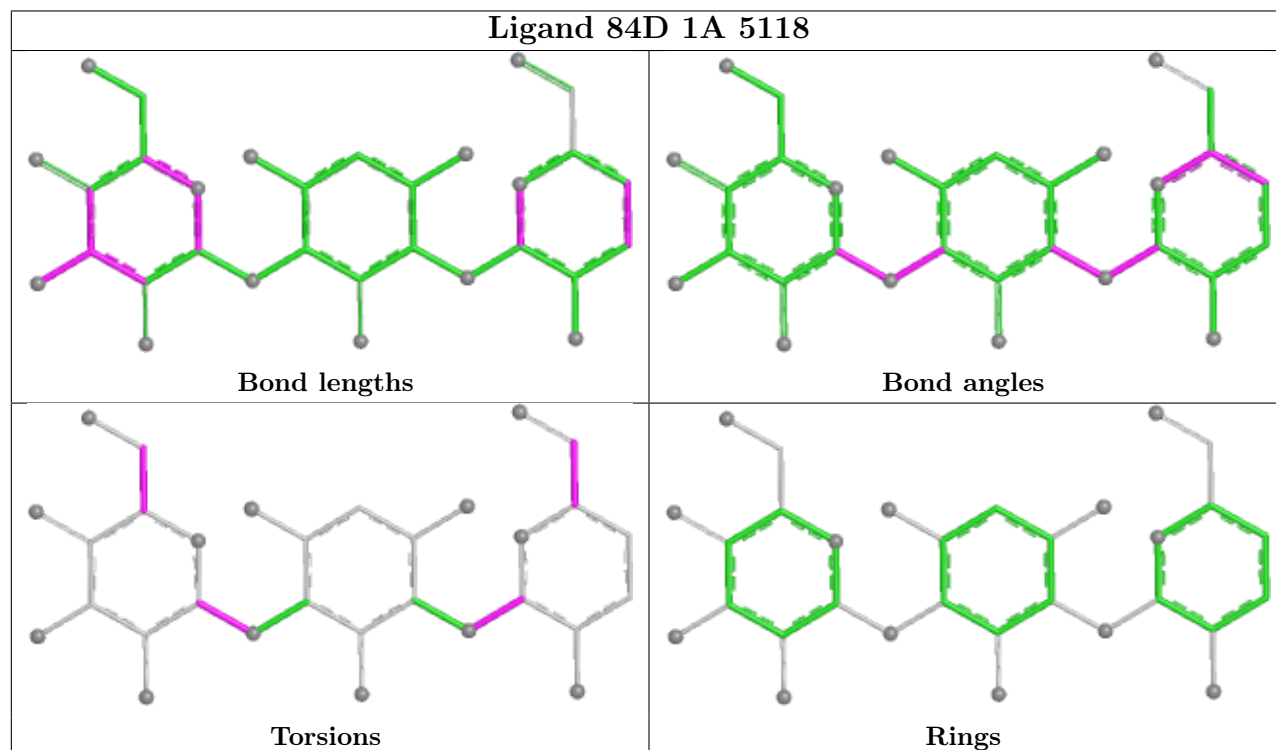
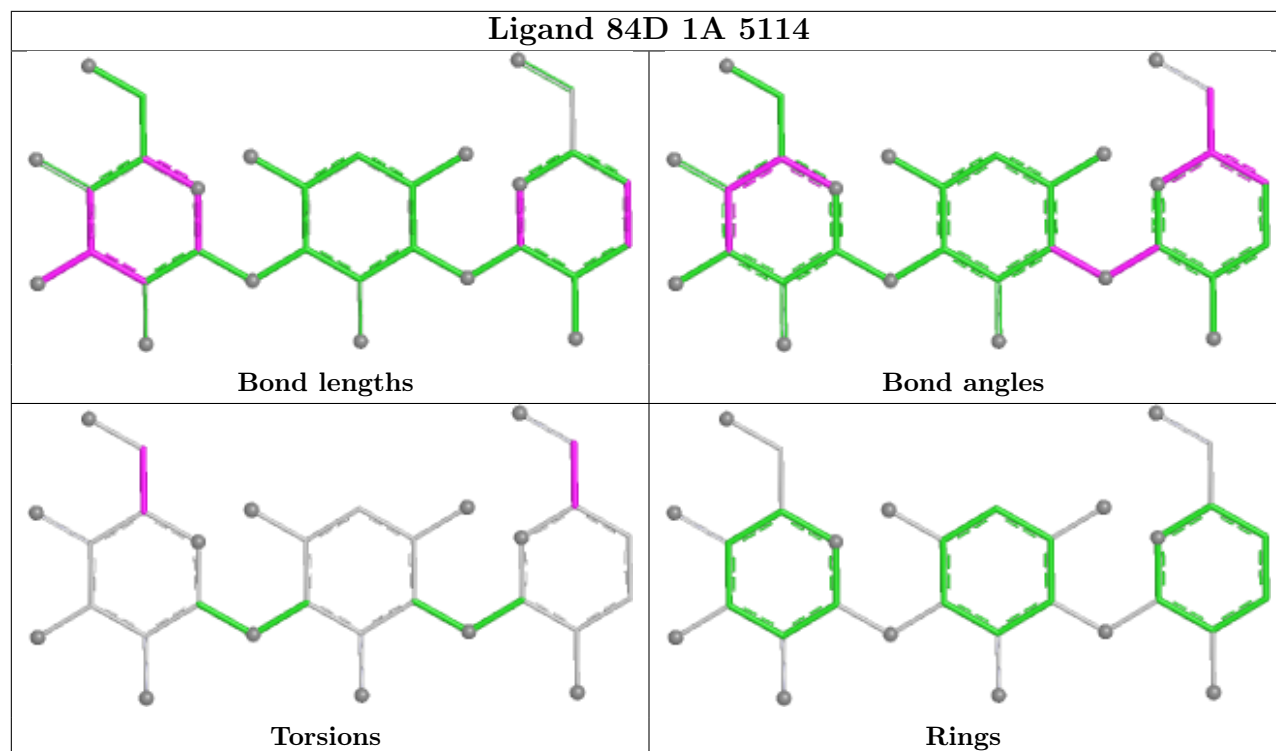
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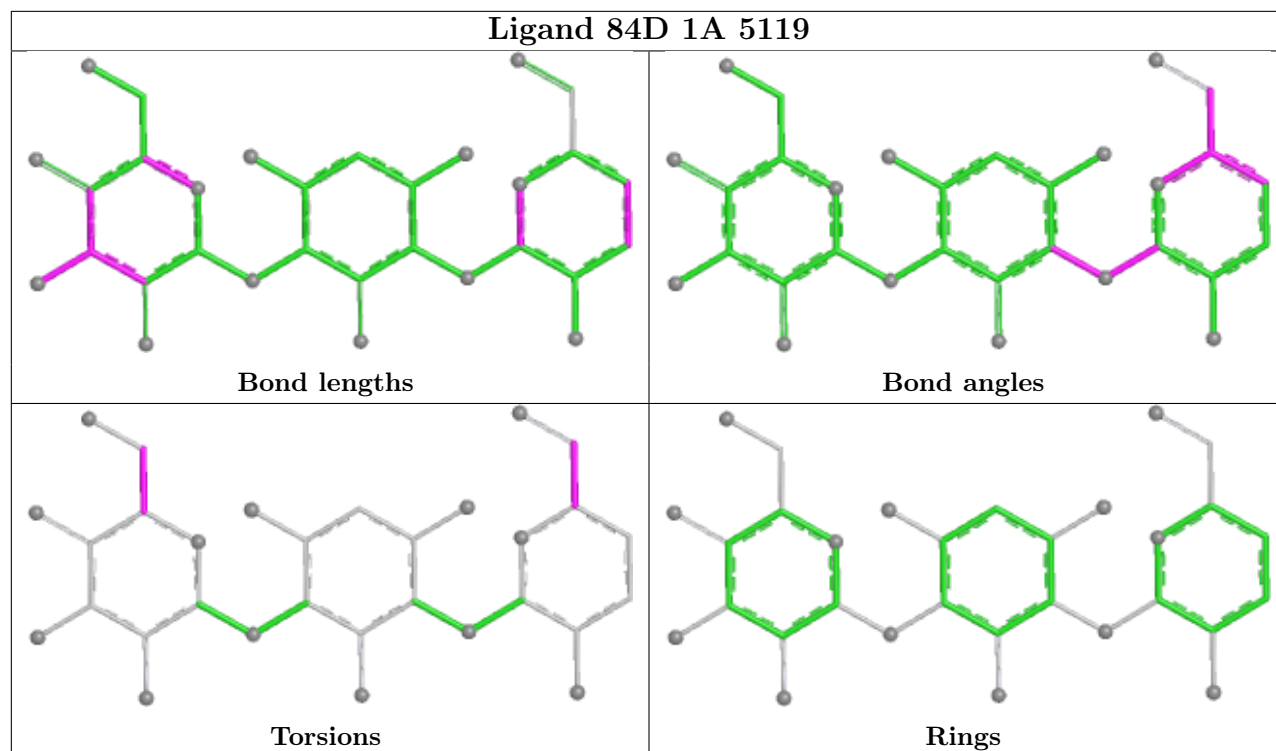
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81  | 1A    | 5107 | 84D  | 1       | 0            |
| 81  | 1A    | 5105 | 84D  | 2       | 0            |
| 81  | 1A    | 5115 | 84D  | 2       | 0            |
| 81  | 1A    | 5101 | 84D  | 1       | 0            |
| 81  | 1A    | 5103 | 84D  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

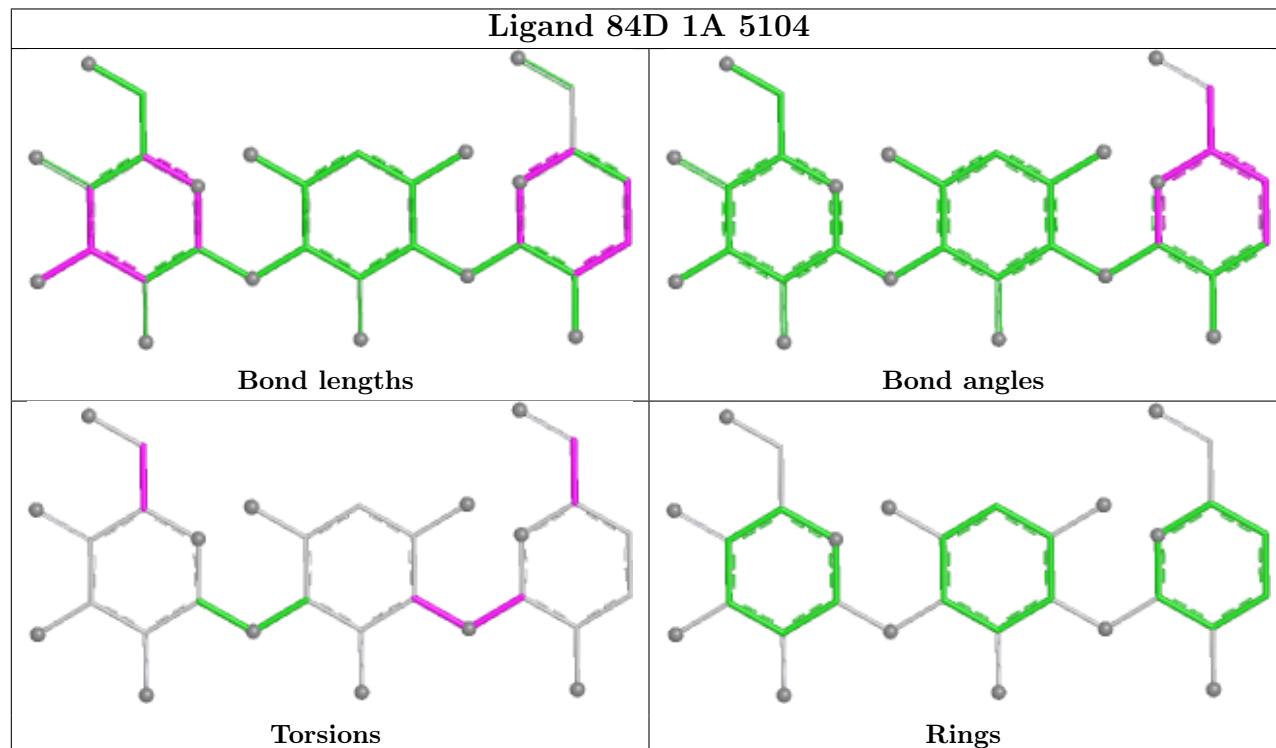




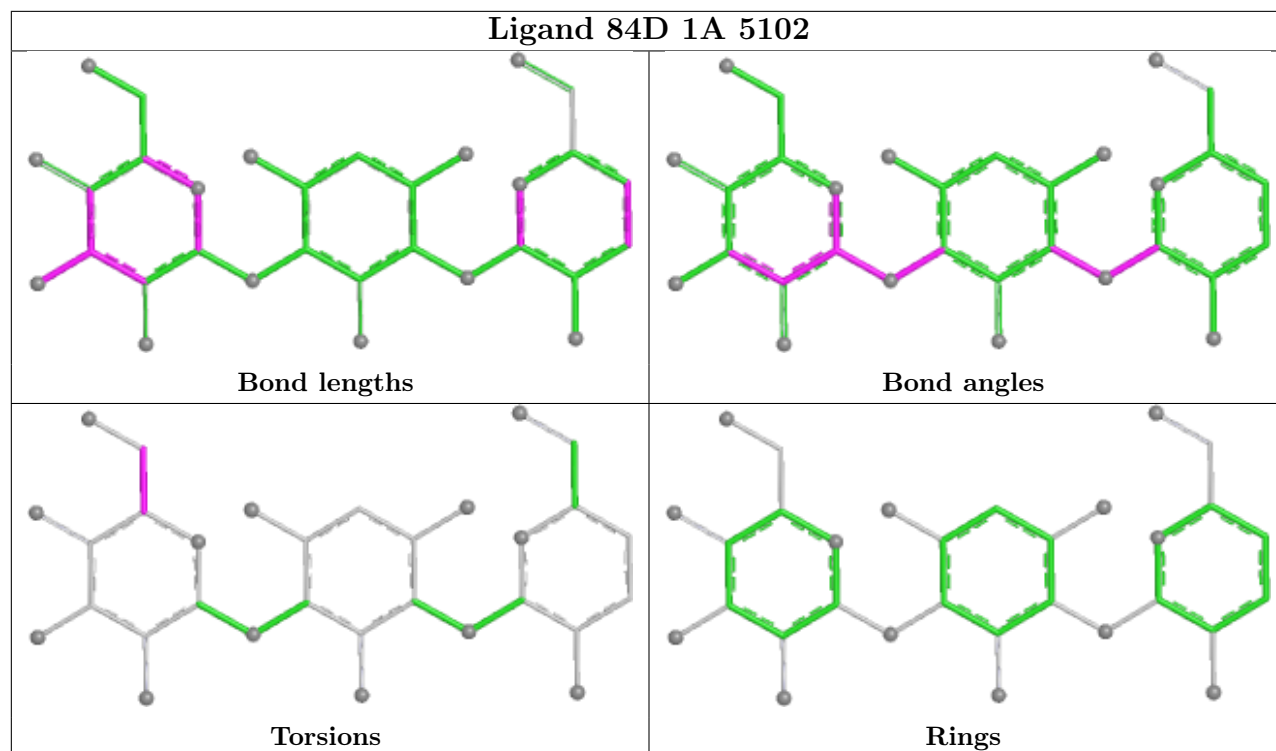
## Ligand 84D 1A 5119



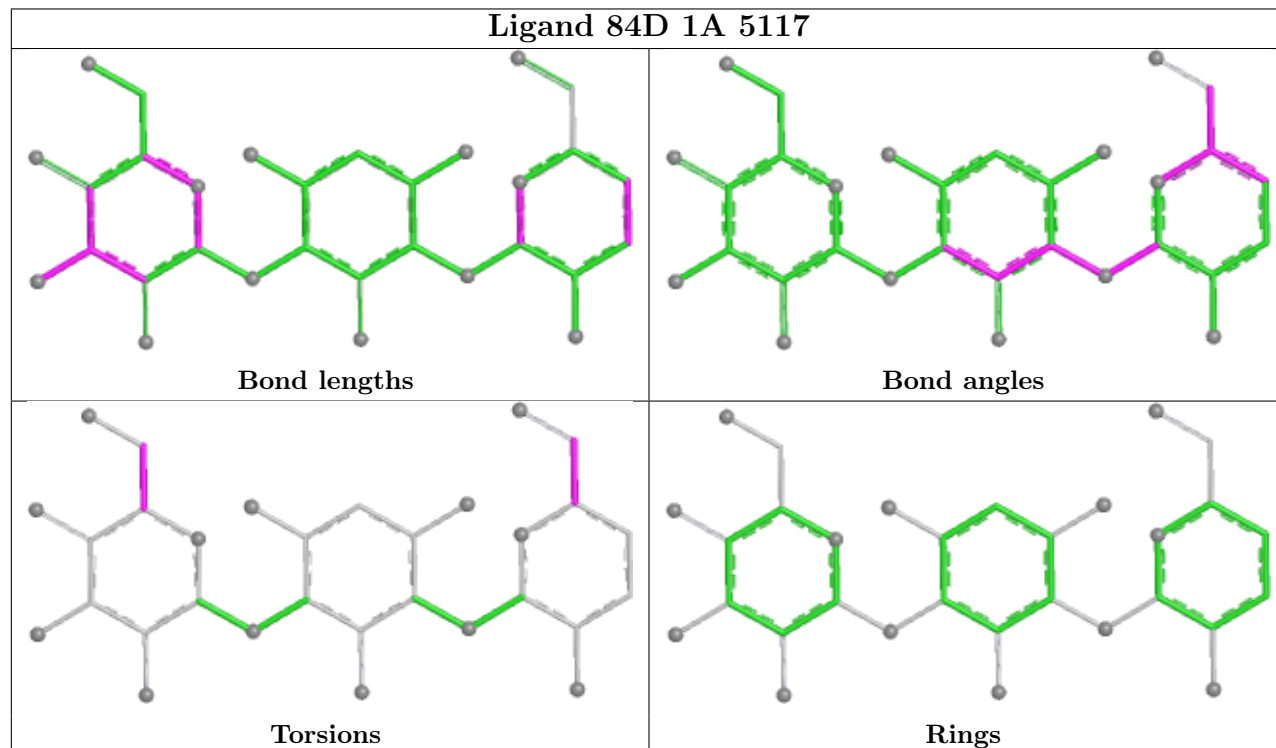
## Ligand 84D 1A 5104

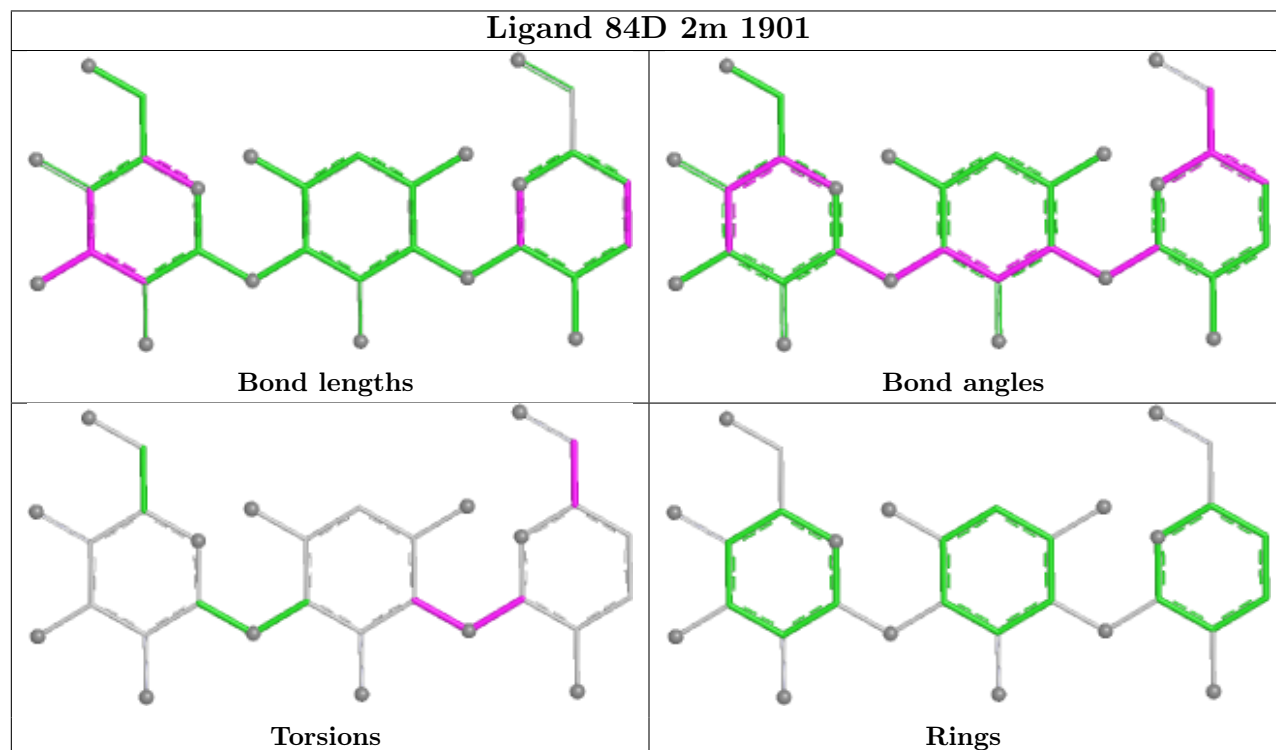
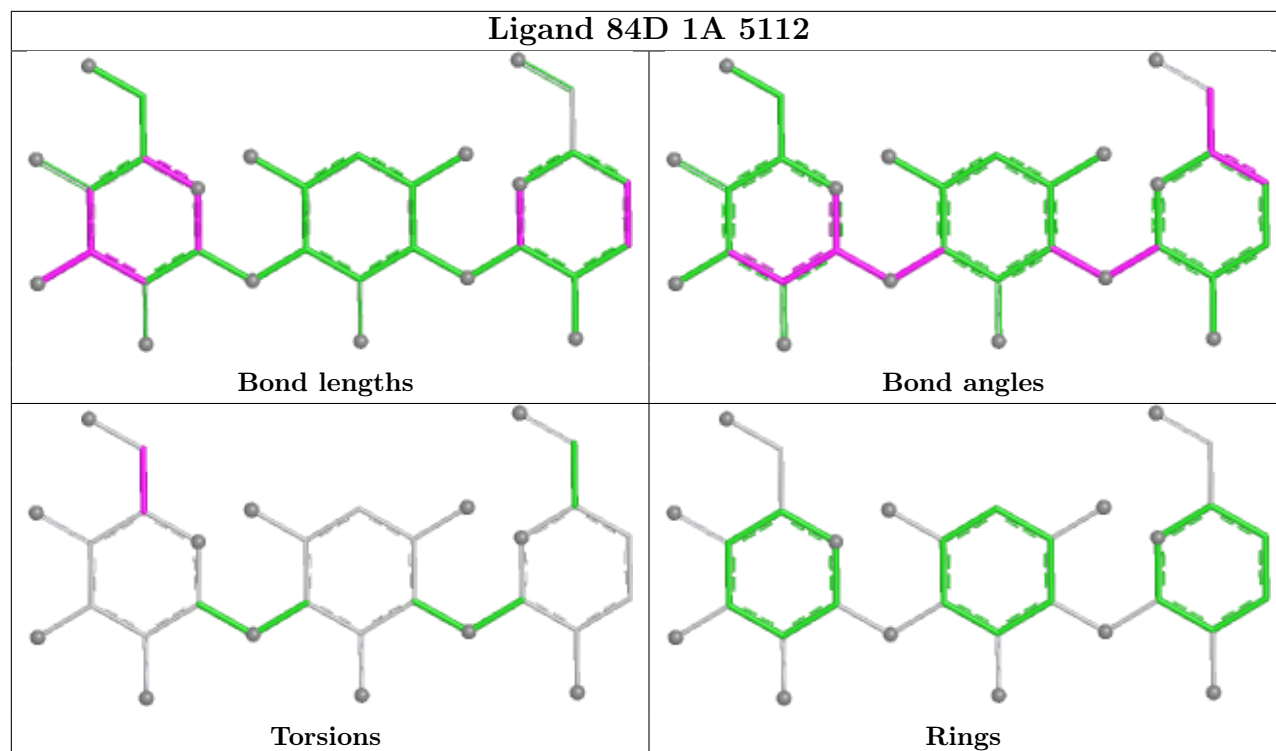


## Ligand 84D 1A 5102

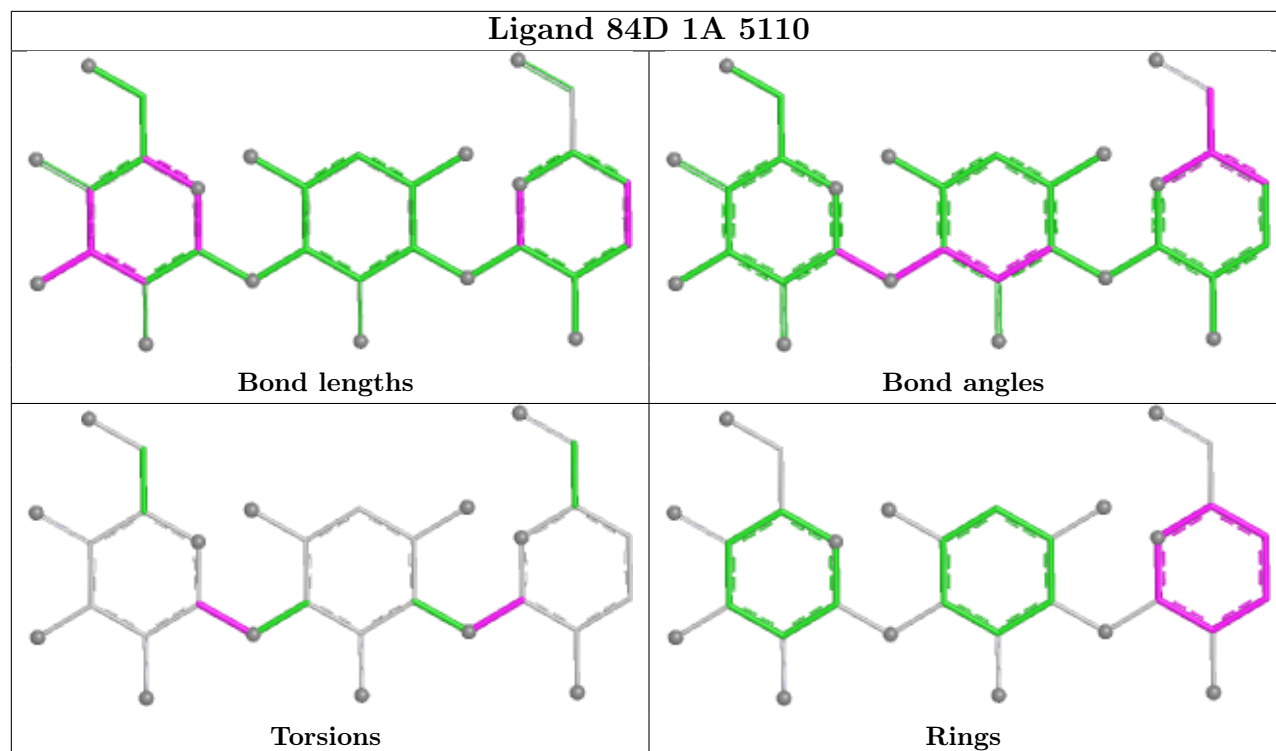


## Ligand 84D 1A 5117

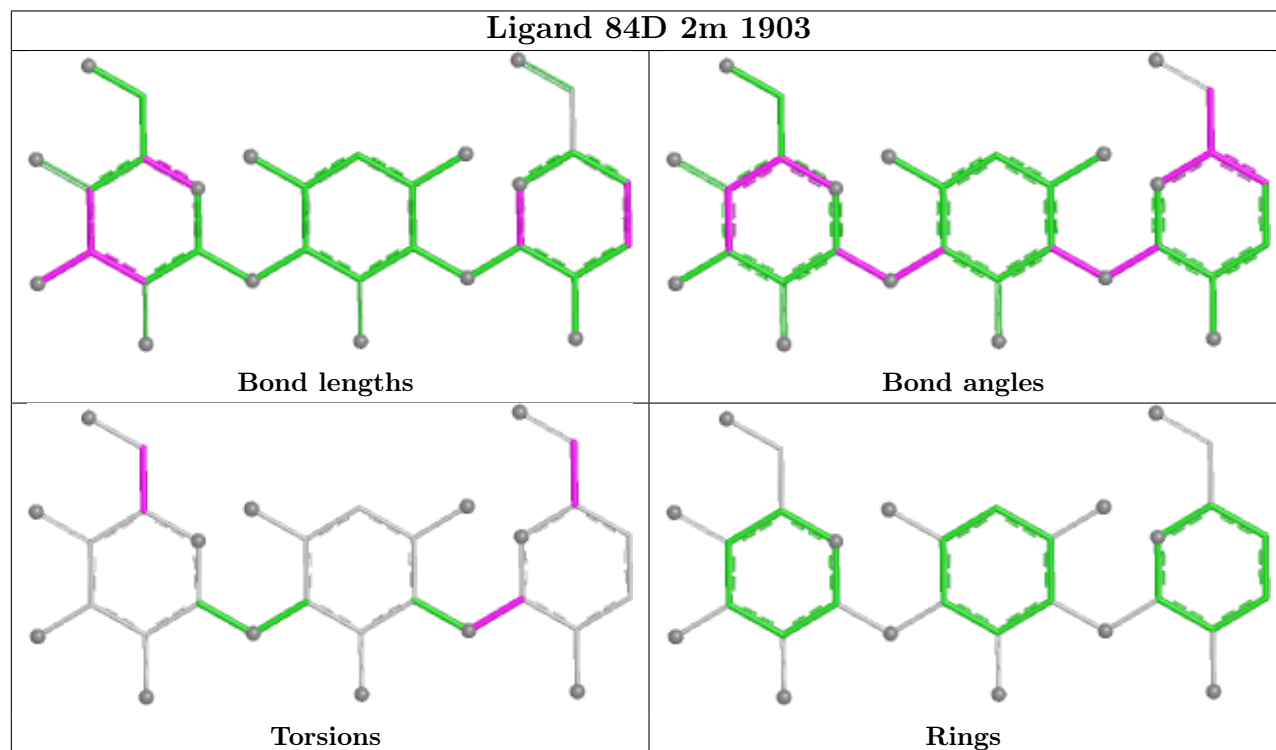




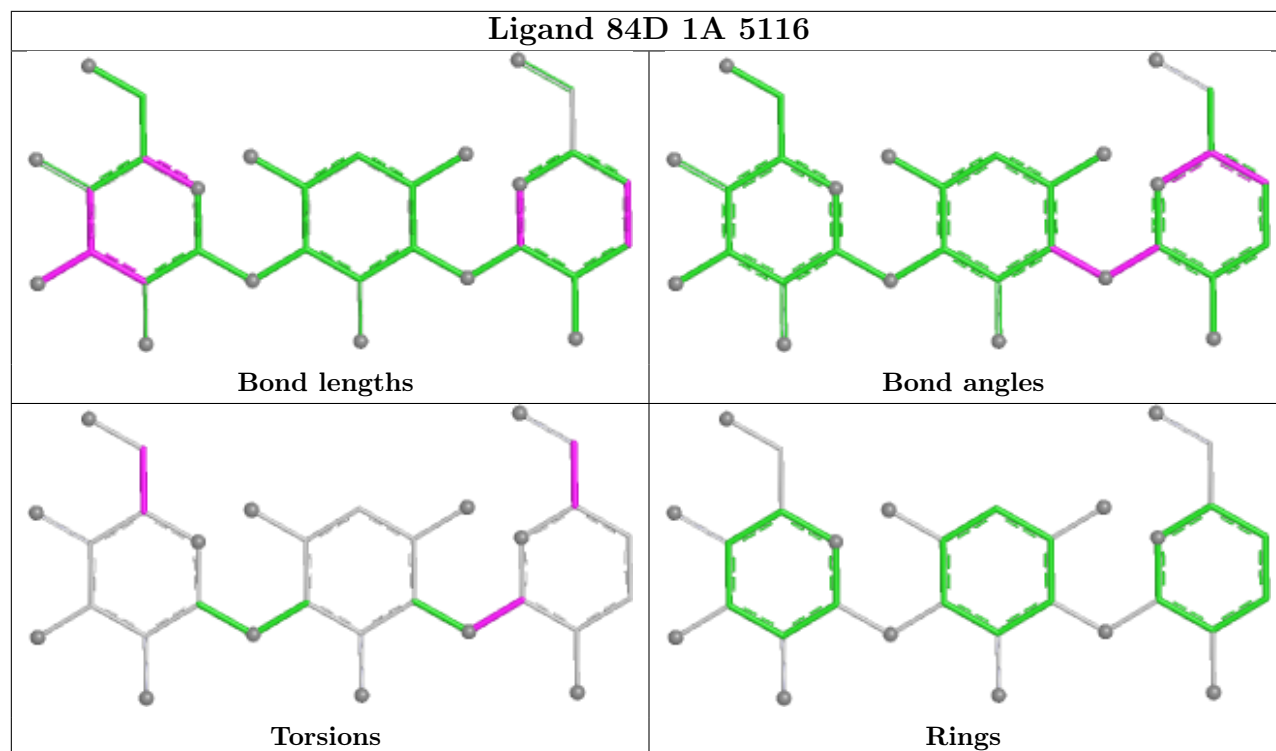
## Ligand 84D 1A 5110



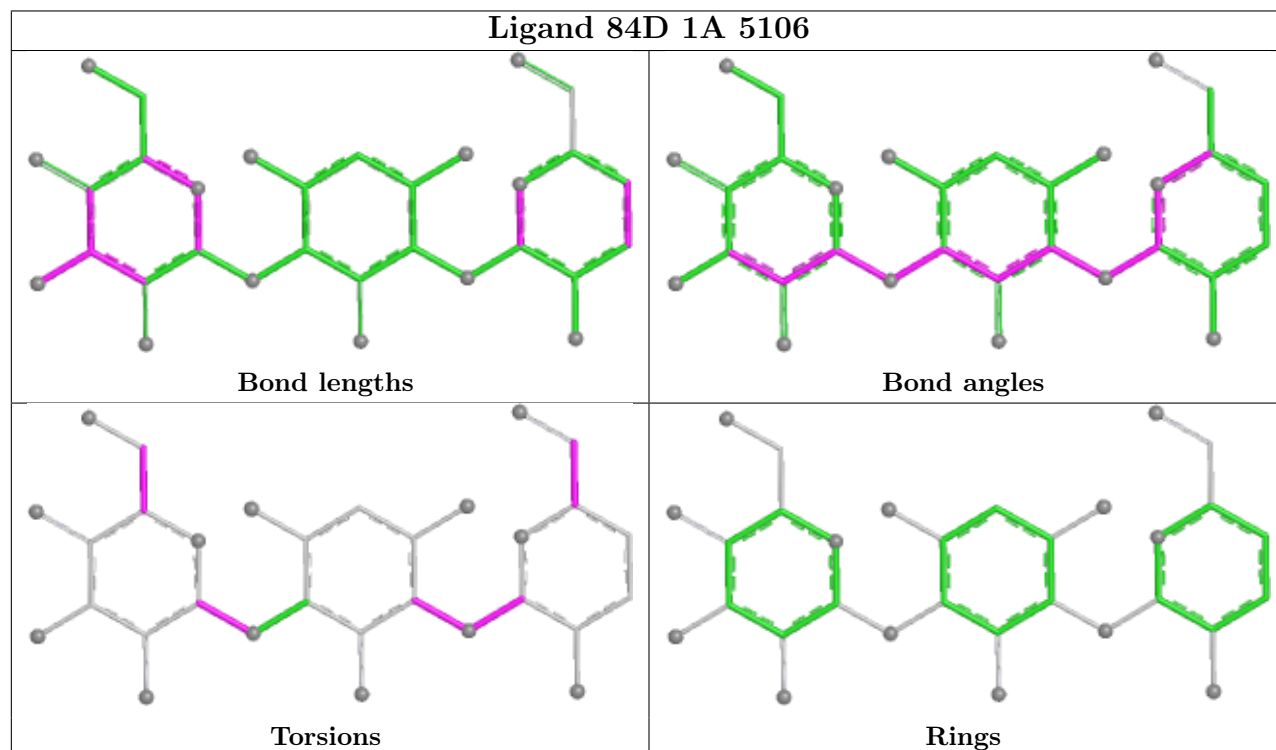
## Ligand 84D 2m 1903



## Ligand 84D 1A 5116

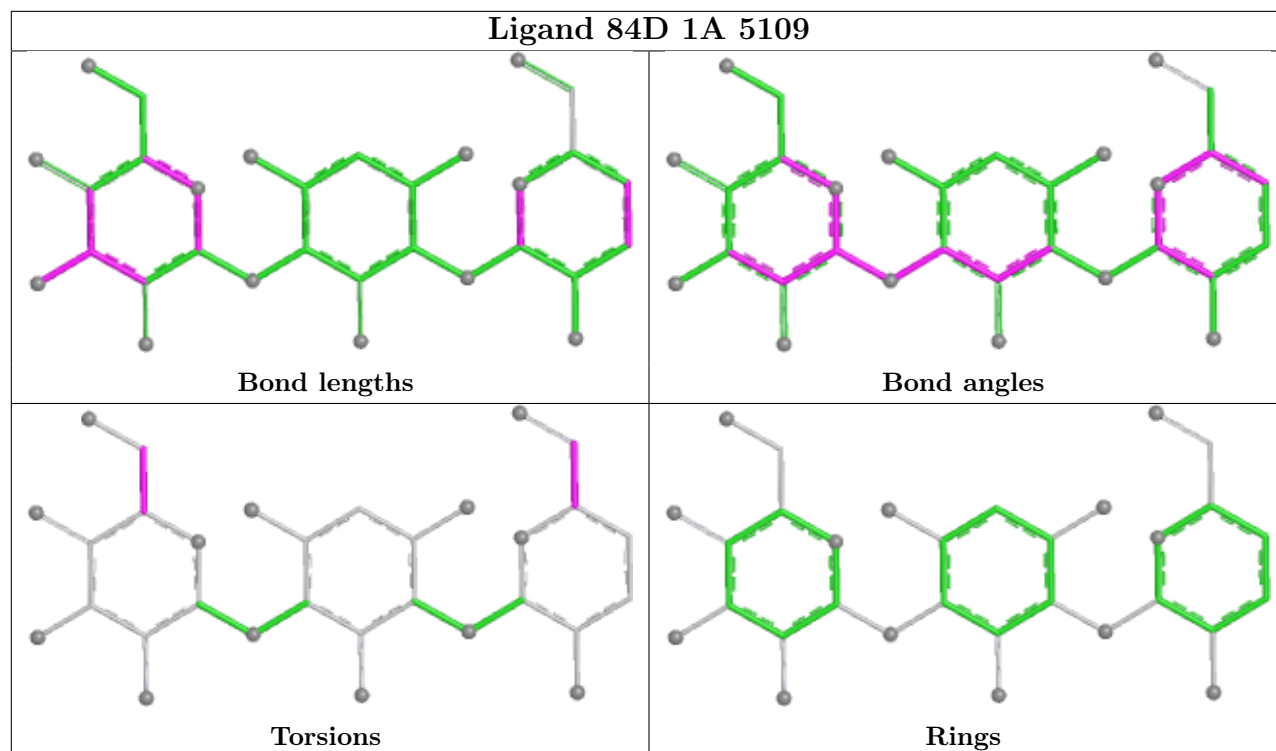


## Ligand 84D 1A 5106

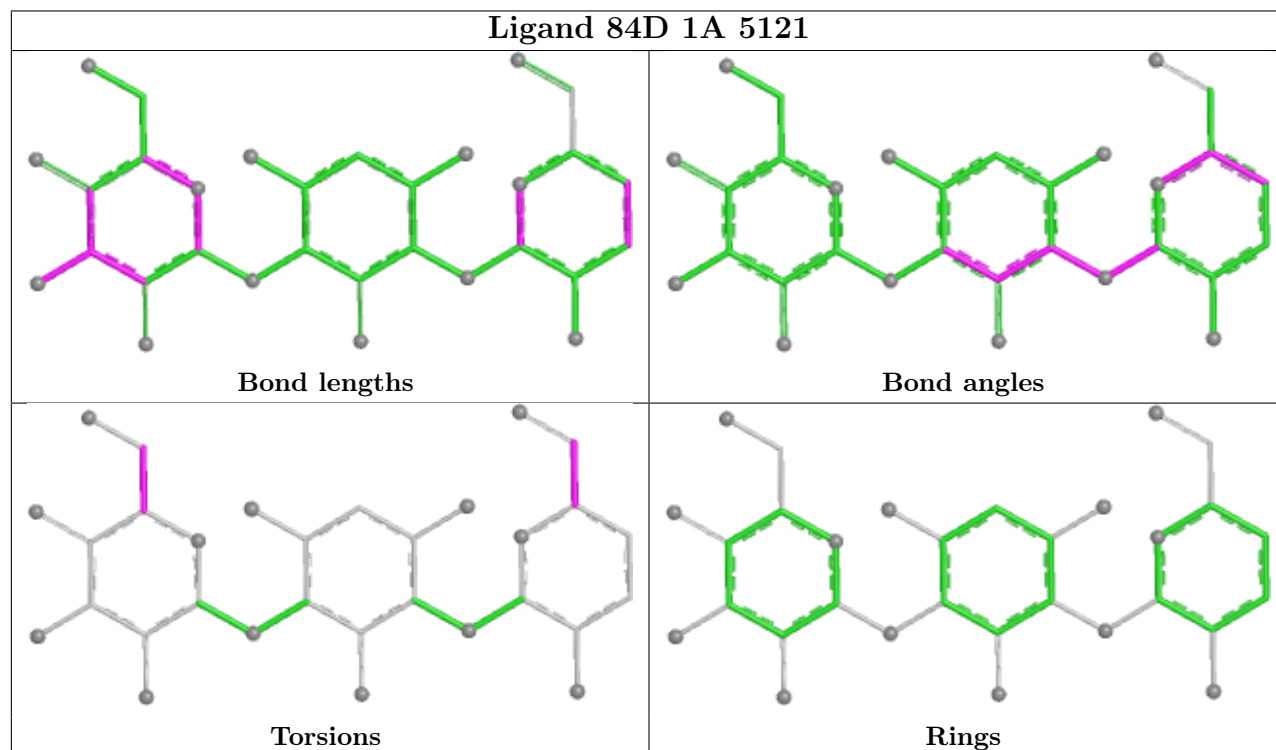


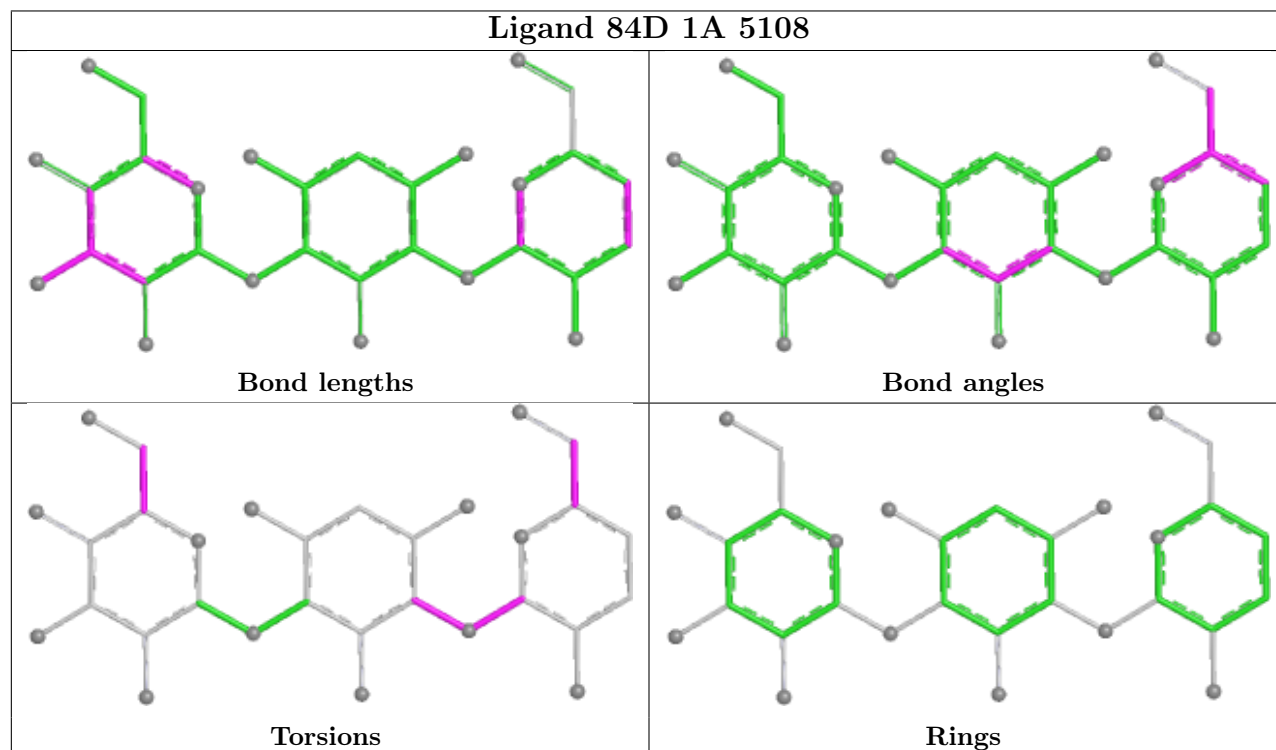
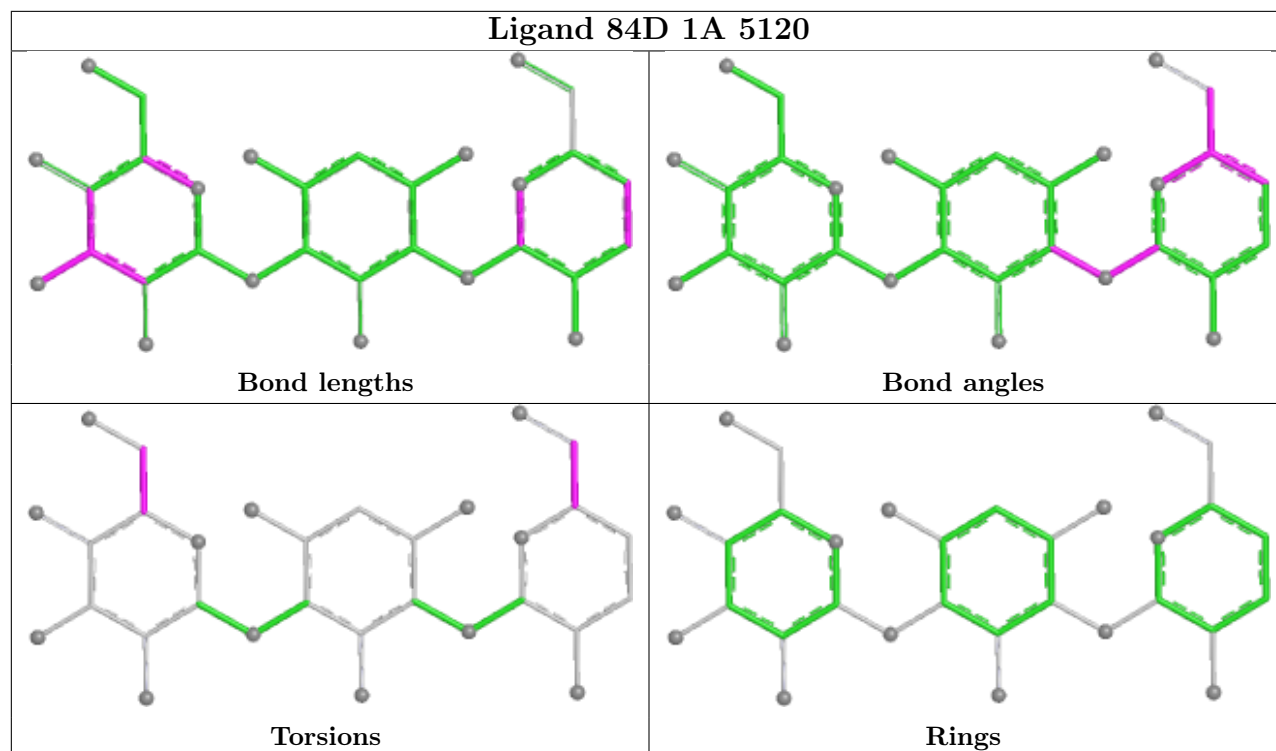


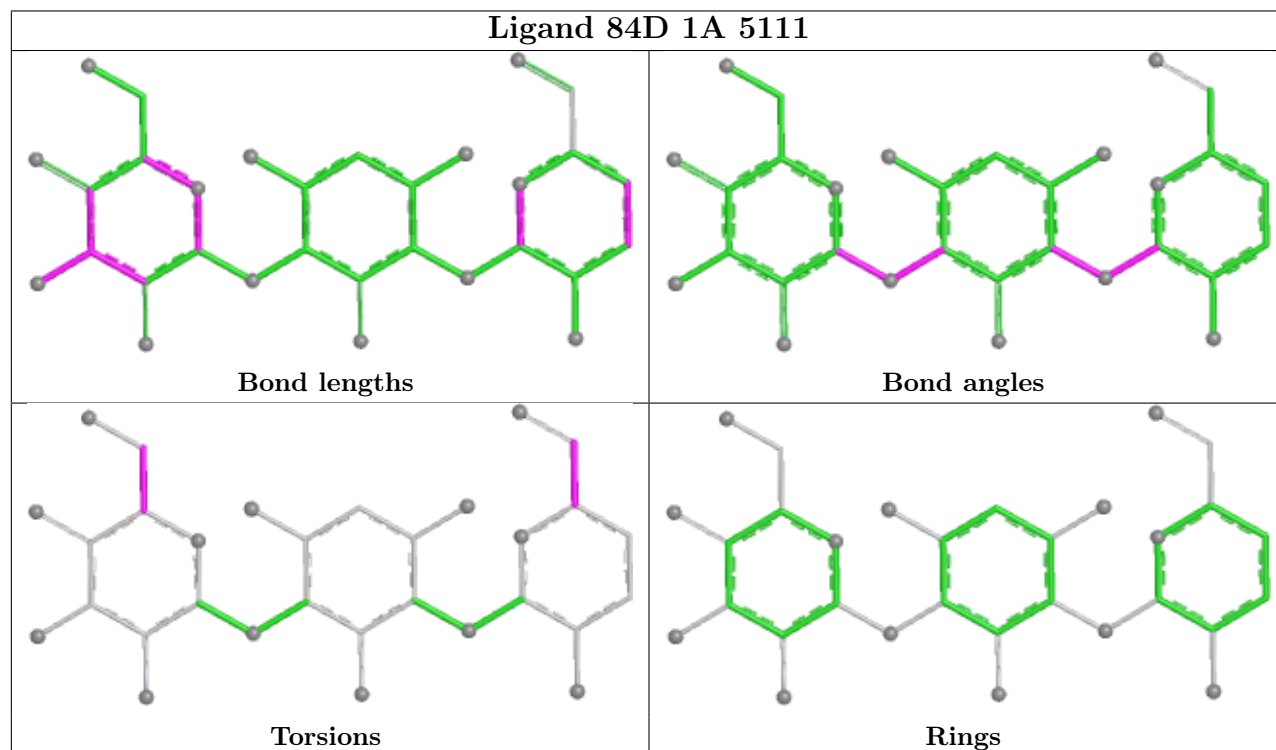
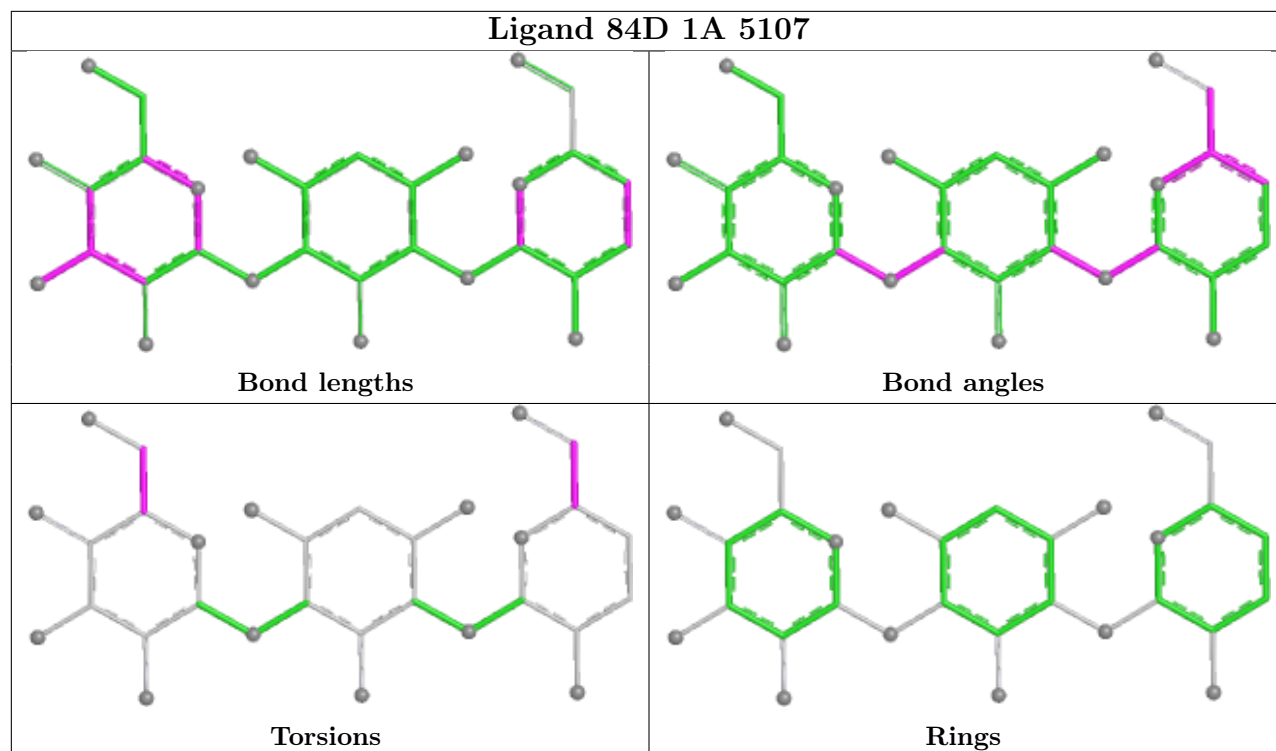
## Ligand 84D 1A 5109



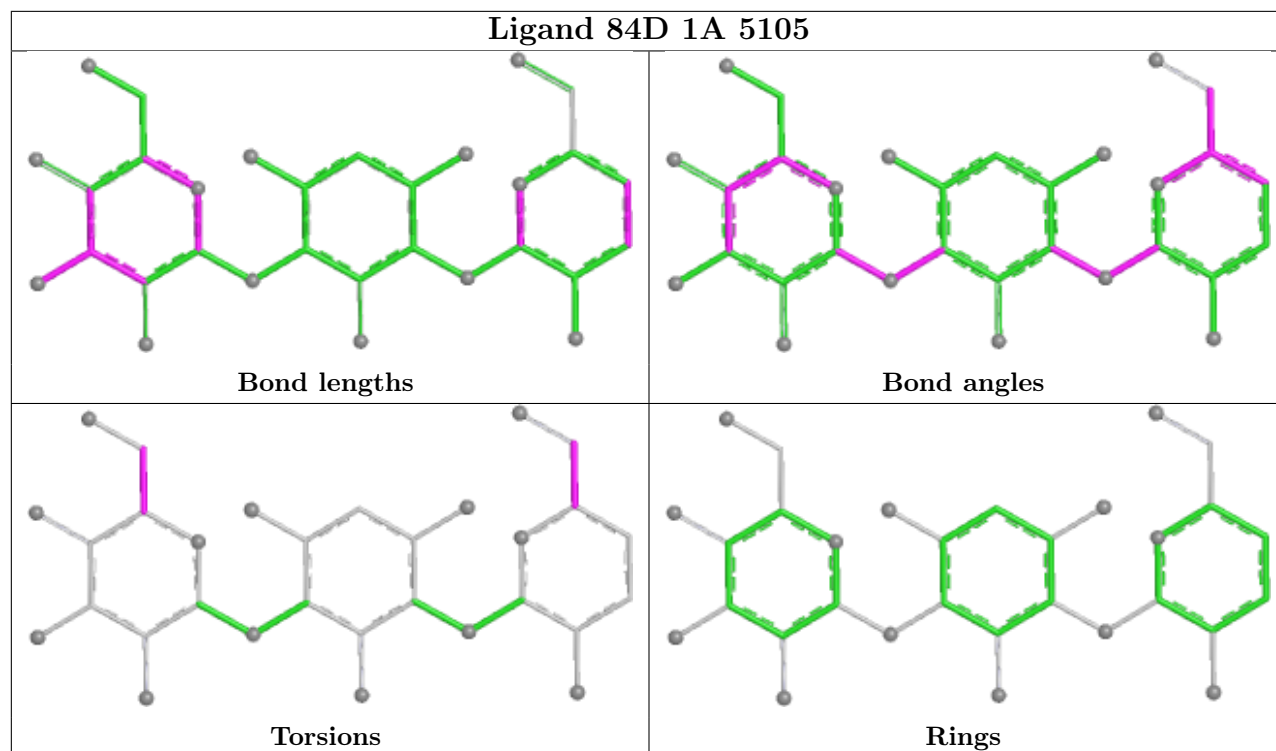
## Ligand 84D 1A 5121



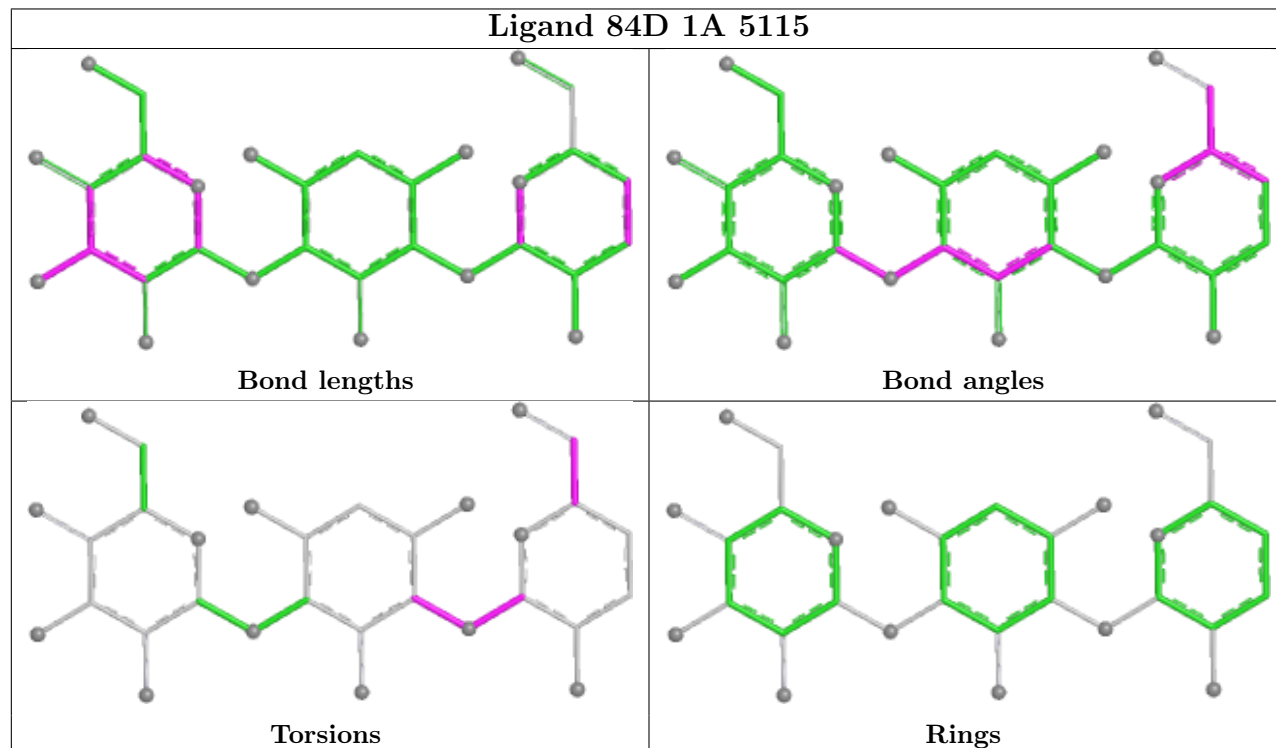


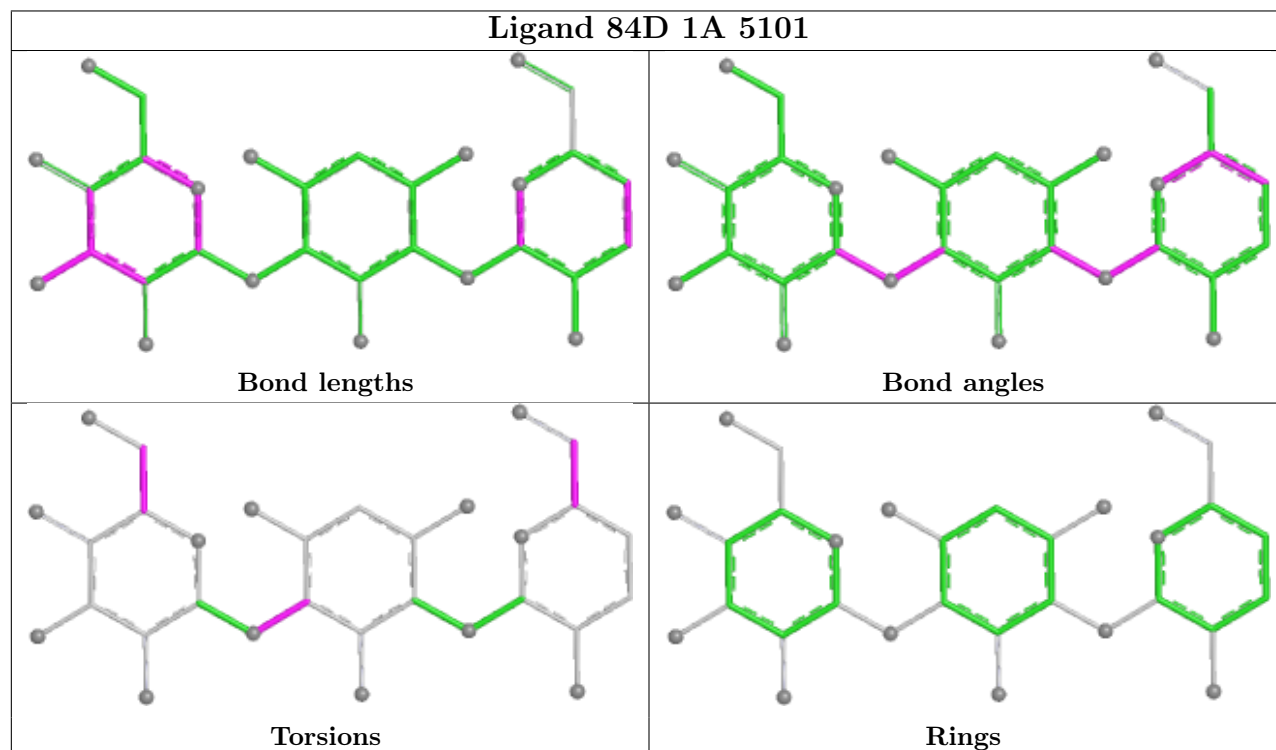
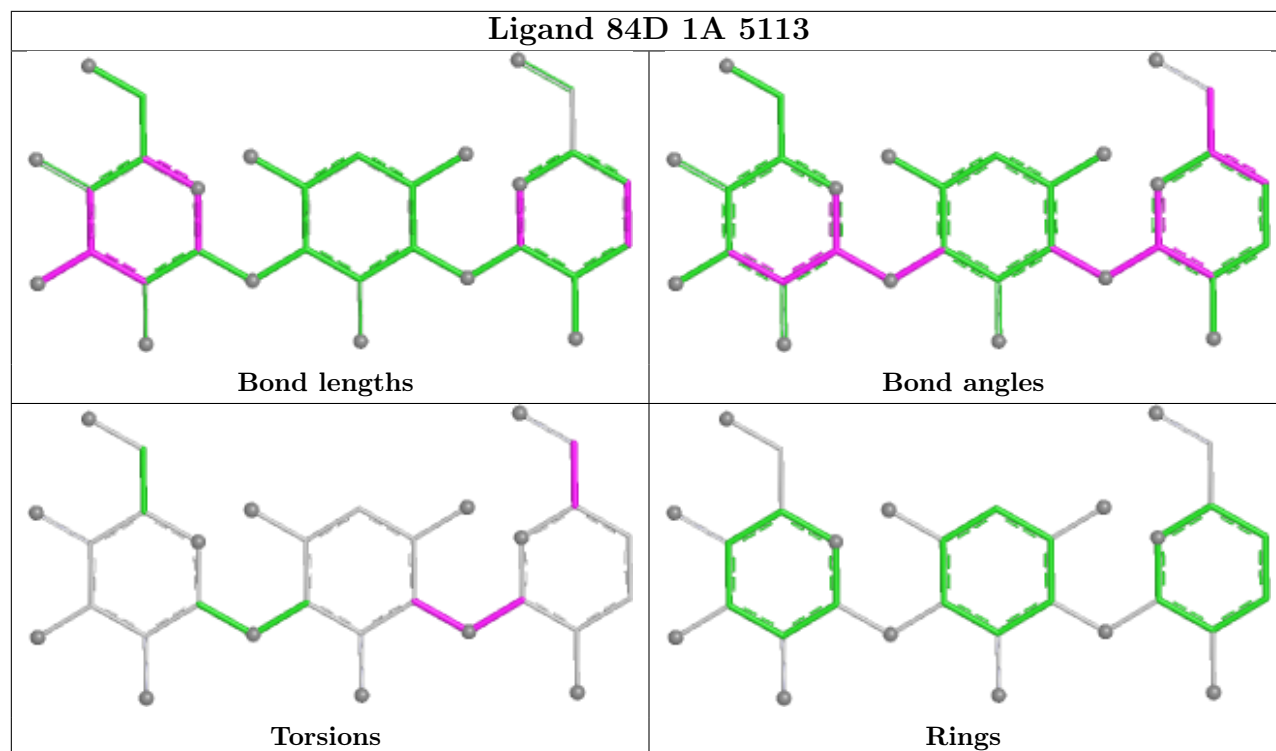


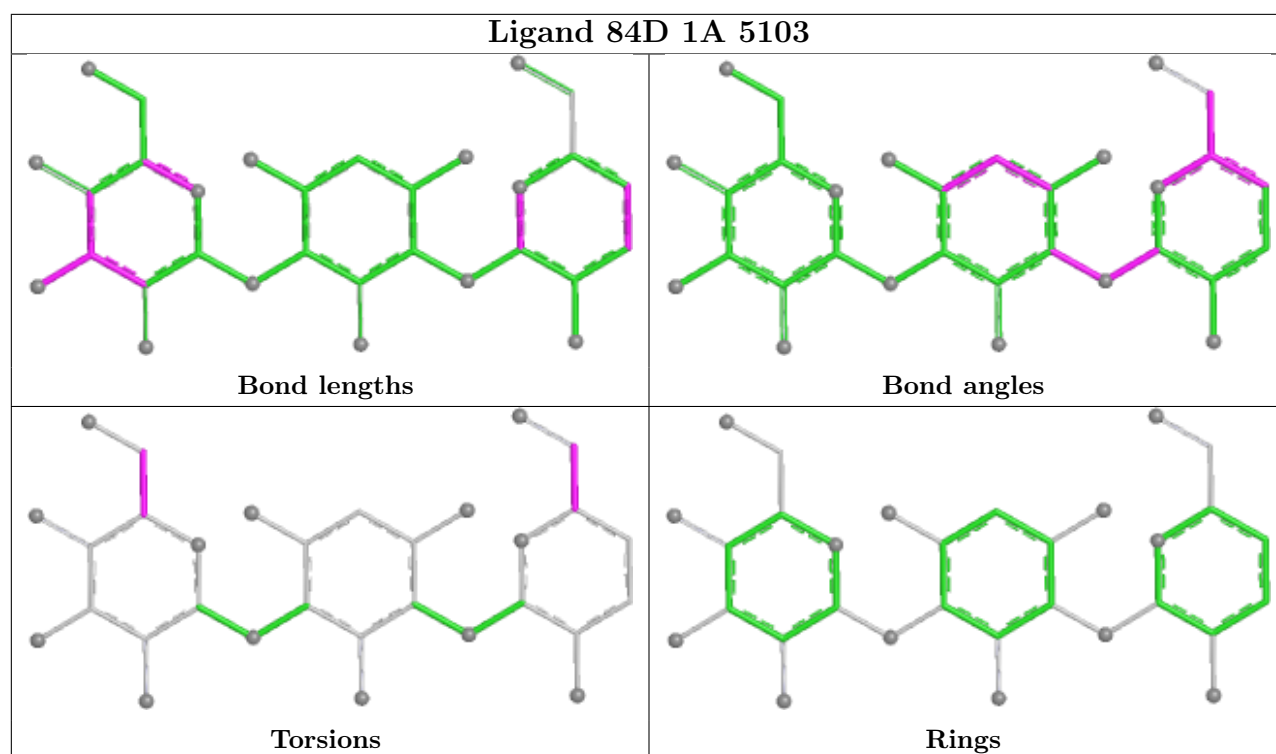
## Ligand 84D 1A 5105



## Ligand 84D 1A 5115







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

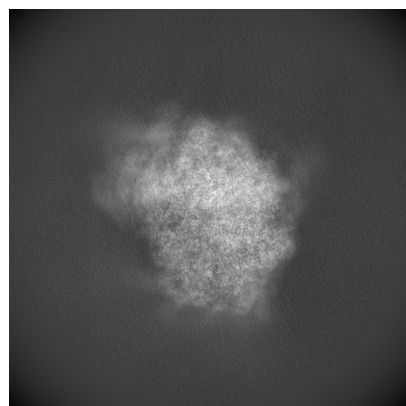
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35413. These allow visual inspection of the internal detail of the map and identification of artifacts.

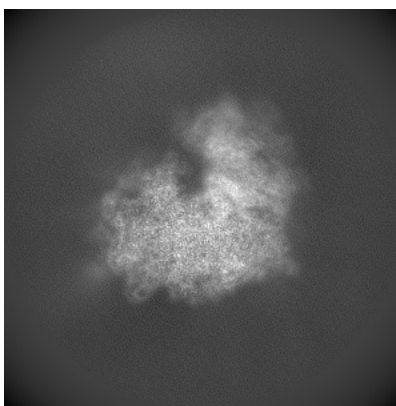
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

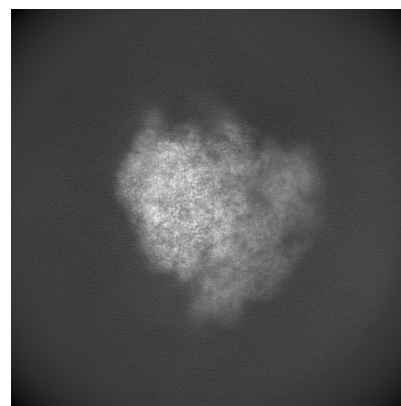
#### 6.1.1 Primary map



X

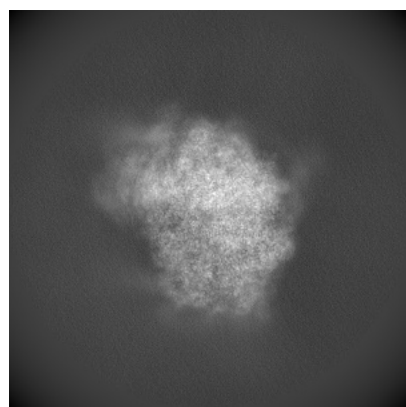


Y

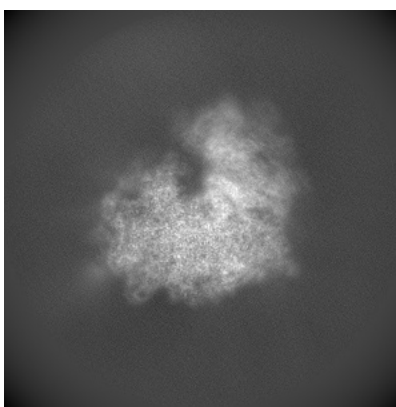


Z

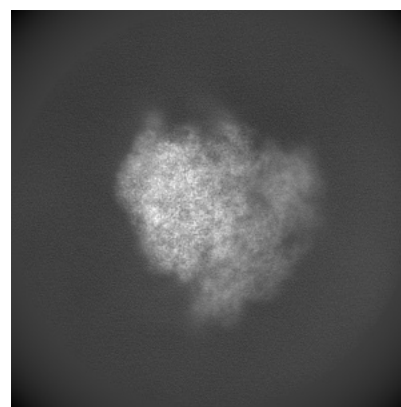
#### 6.1.2 Raw map



X



Y



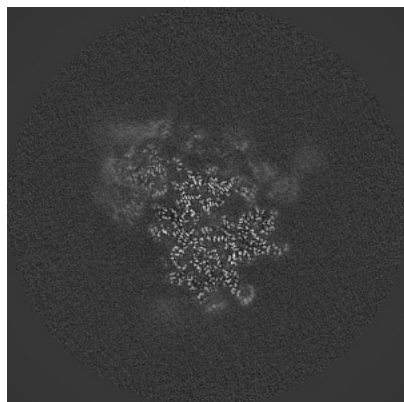
Z

The images above show the map projected in three orthogonal directions.

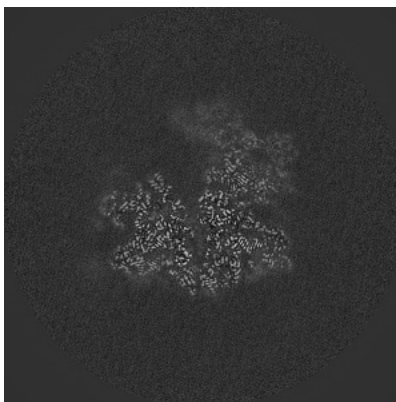


## 6.2 Central slices [i](#)

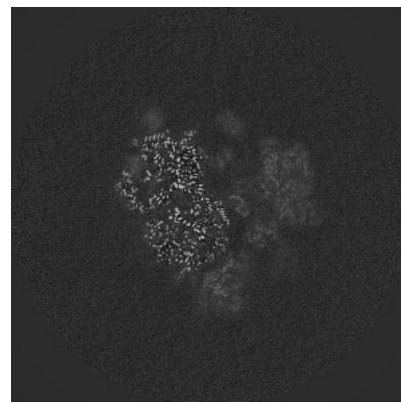
### 6.2.1 Primary map



X Index: 320

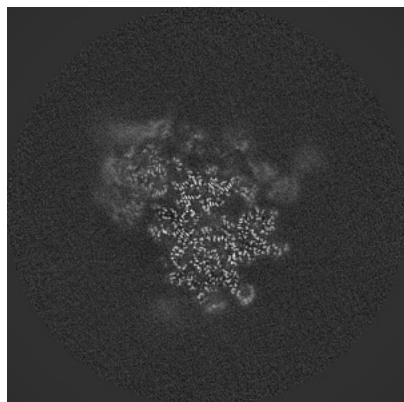


Y Index: 320

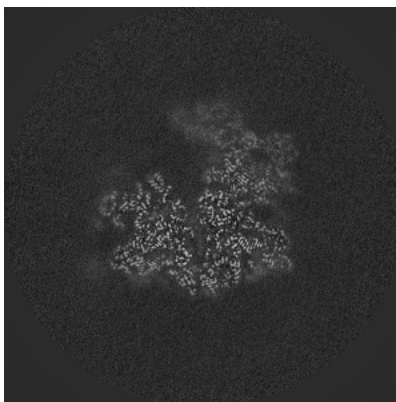


Z Index: 320

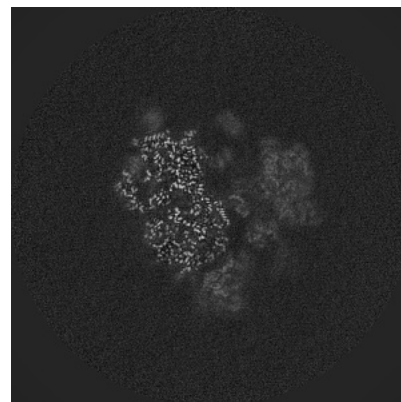
### 6.2.2 Raw map



X Index: 320



Y Index: 320



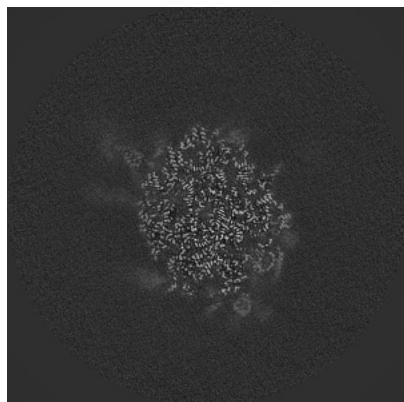
Z Index: 320

The images above show central slices of the map in three orthogonal directions.

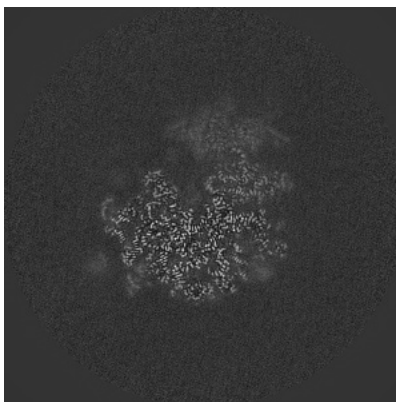


## 6.3 Largest variance slices [i](#)

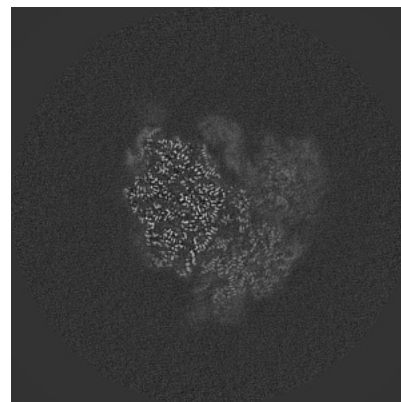
### 6.3.1 Primary map



X Index: 288

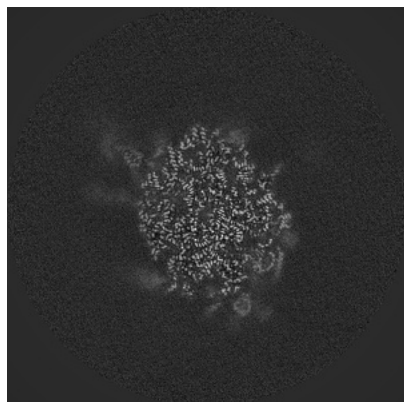


Y Index: 339

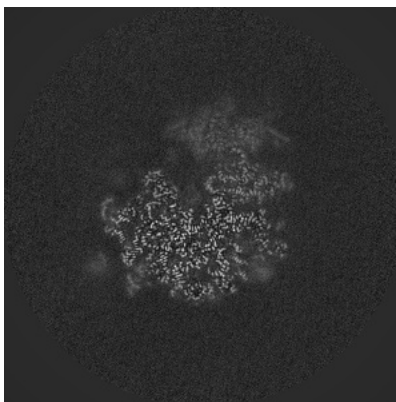


Z Index: 350

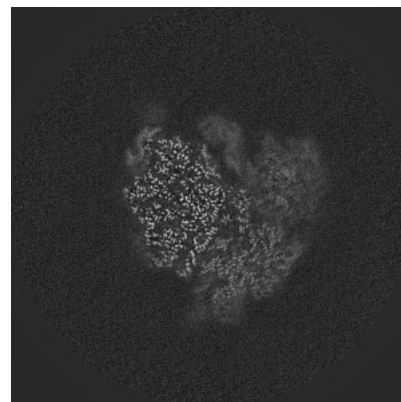
### 6.3.2 Raw map



X Index: 288



Y Index: 339

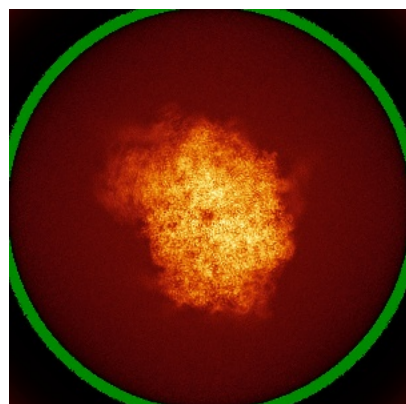


Z Index: 350

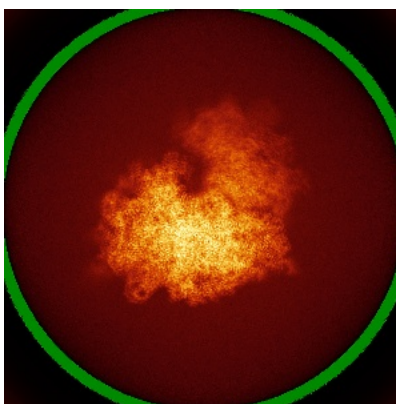
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

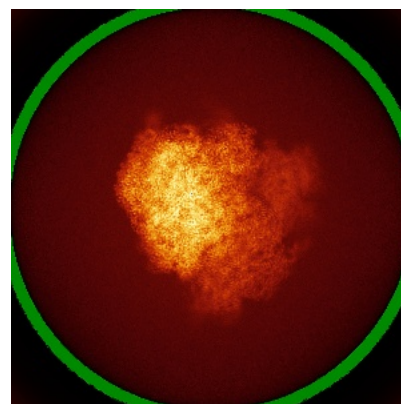
### 6.4.1 Primary map



X

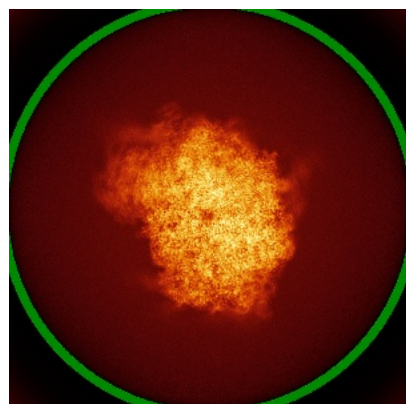


Y

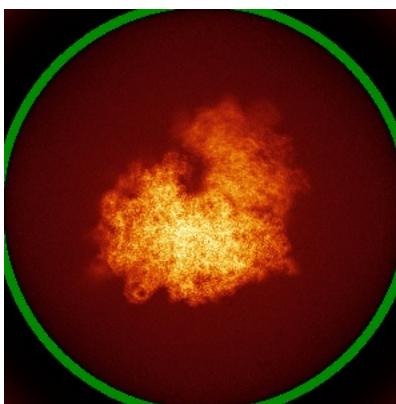


Z

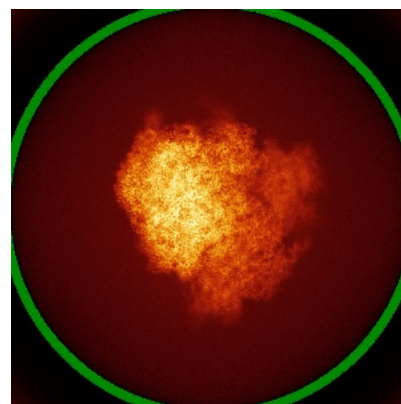
### 6.4.2 Raw map



X



Y

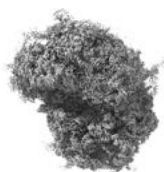


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



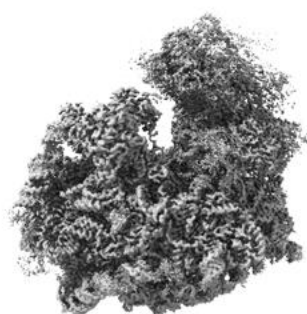
Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

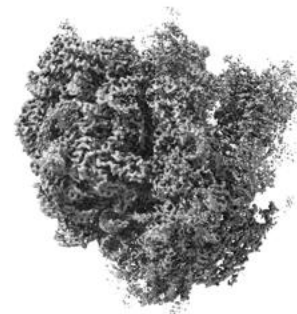
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

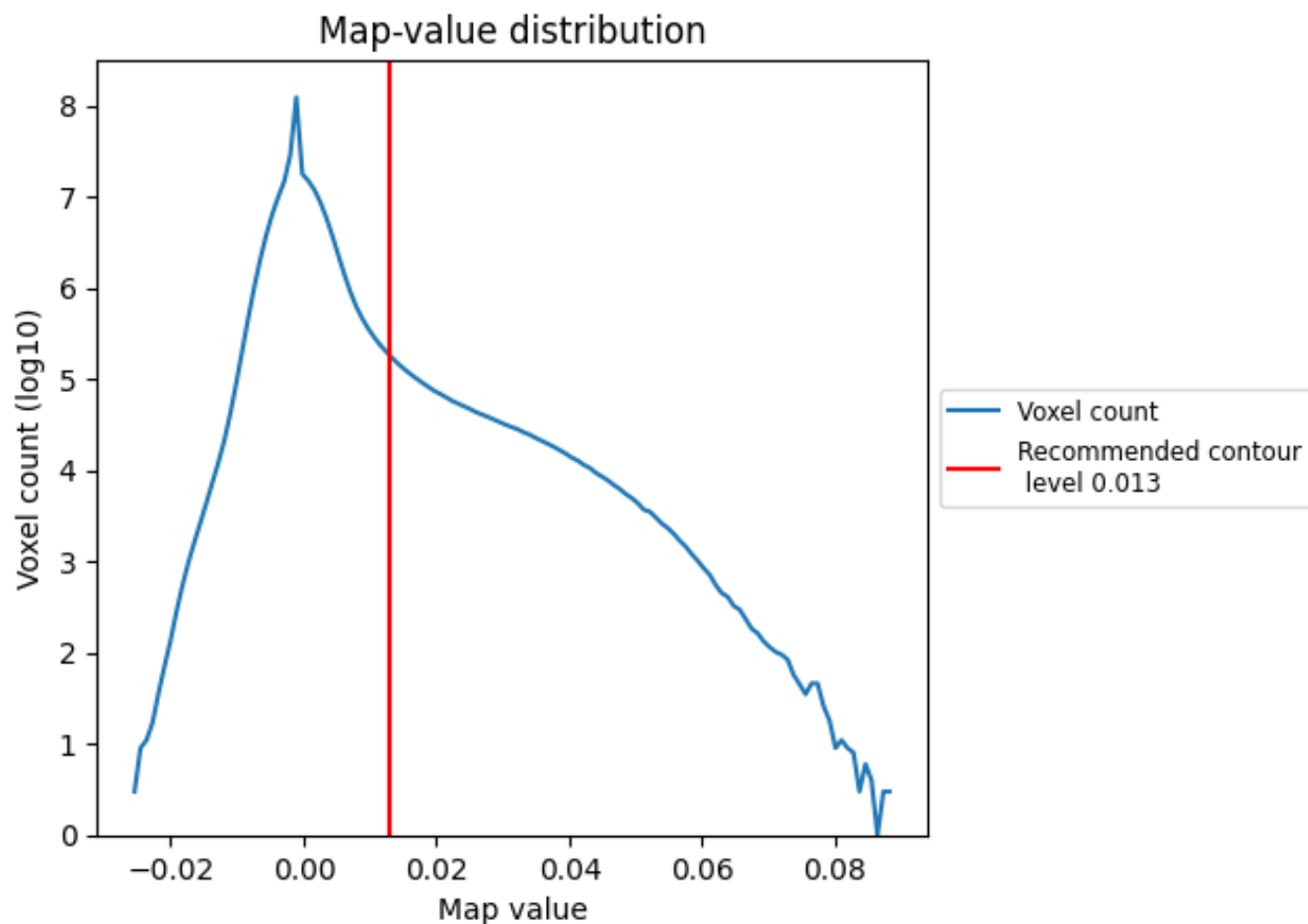
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

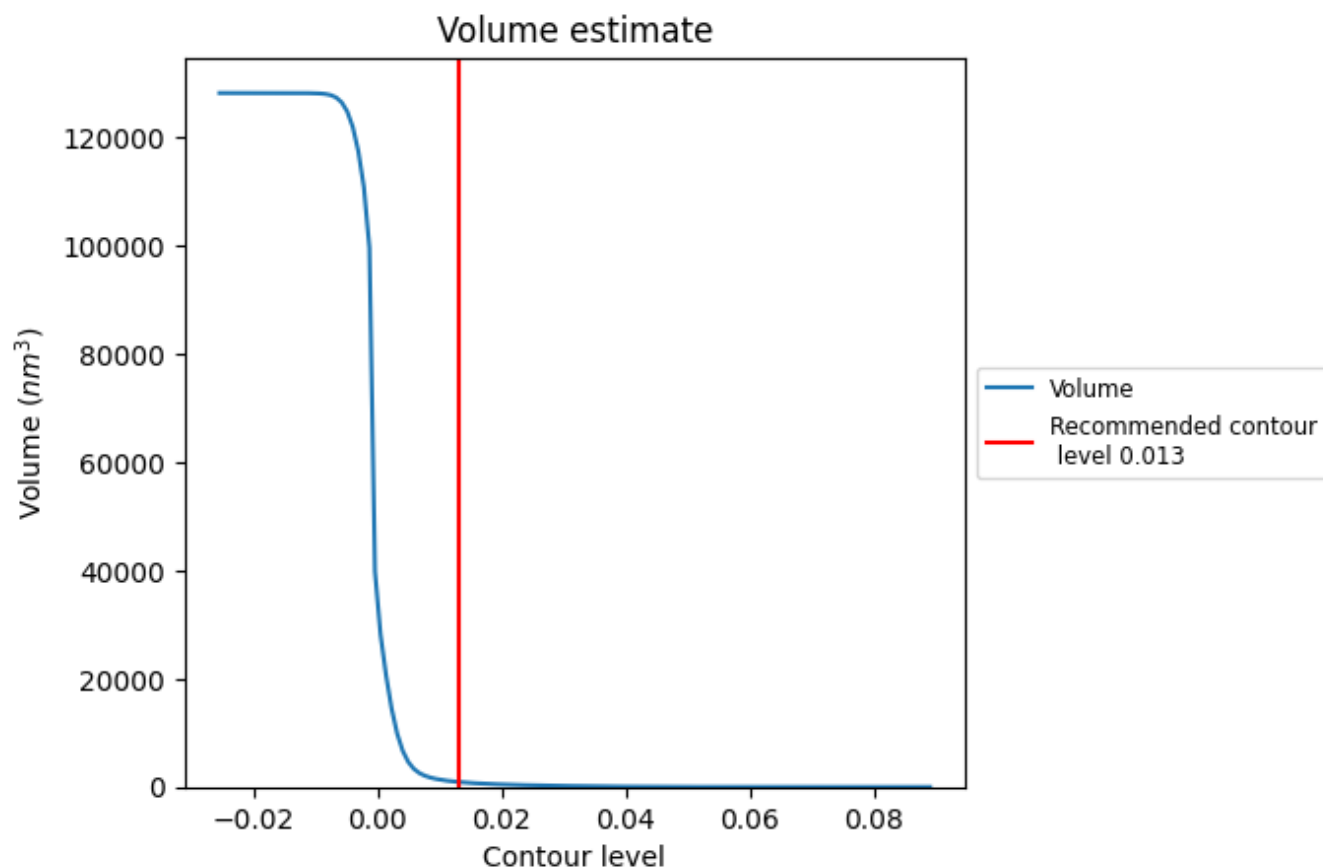
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

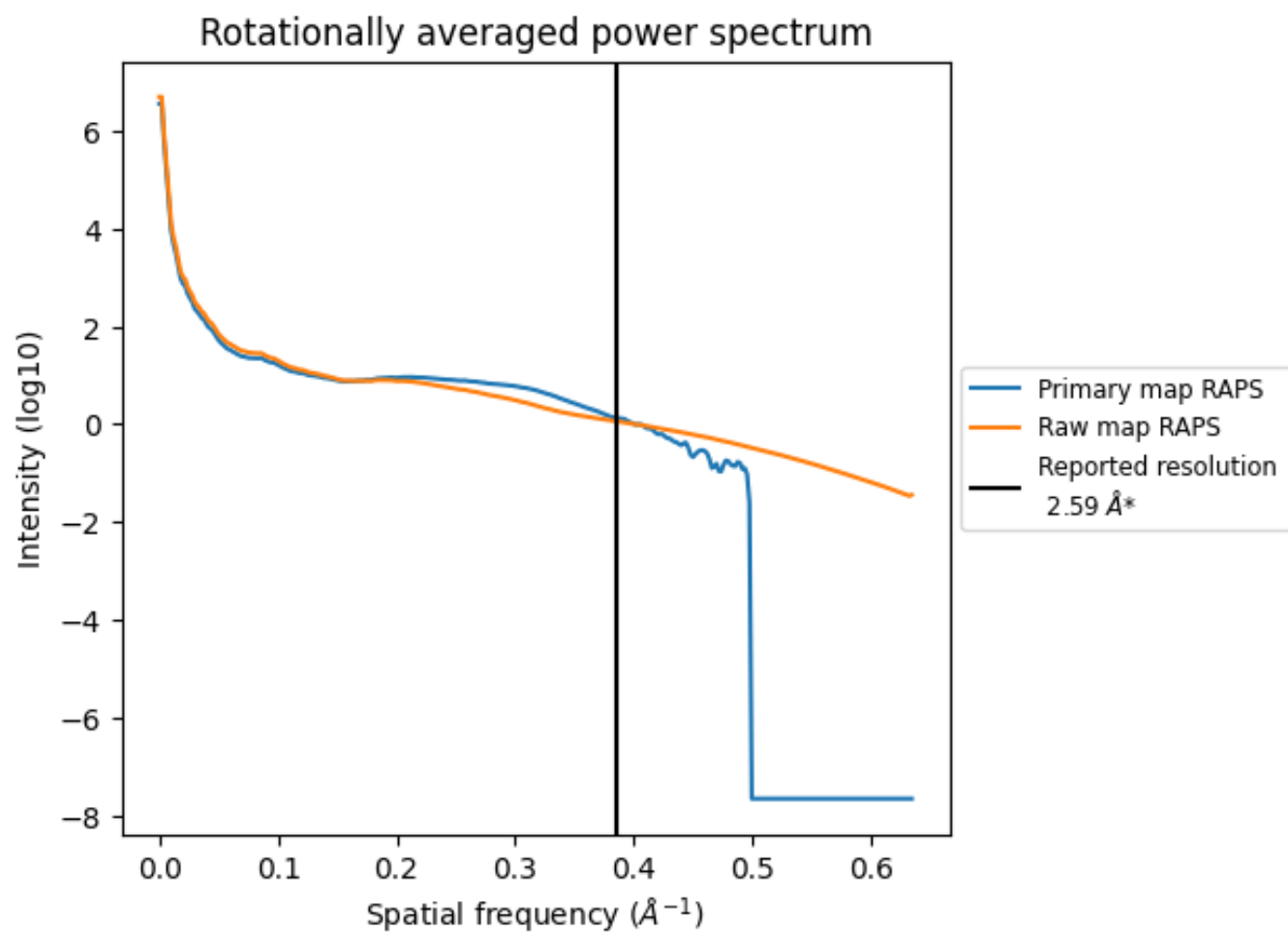
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 927  $\text{nm}^3$ ; this corresponds to an approximate mass of 837 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

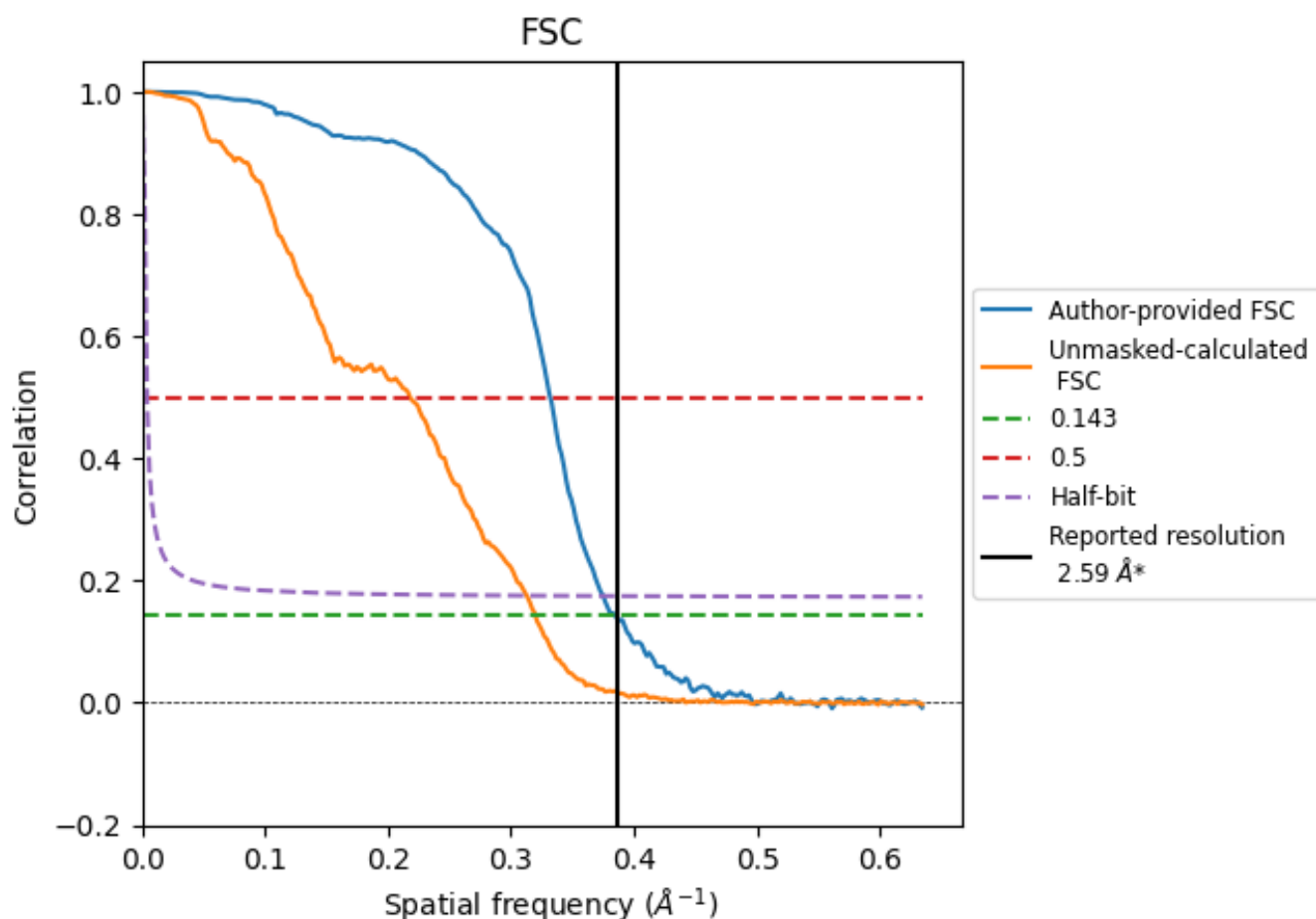


\*Reported resolution corresponds to spatial frequency of 0.386  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.386 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.59                               | -    | -        |
| Author-provided FSC curve | 2.60                               | 3.01 | 2.67     |
| Unmasked-calculated*      | 3.13                               | 4.59 | 3.20     |

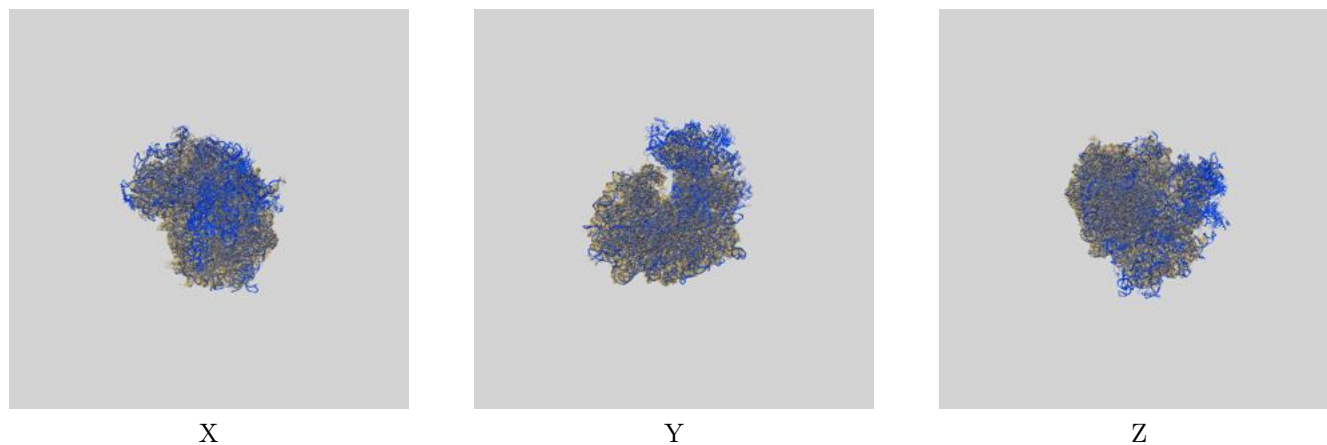
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.59 by more than 10 %



## 9 Map-model fit [i](#)

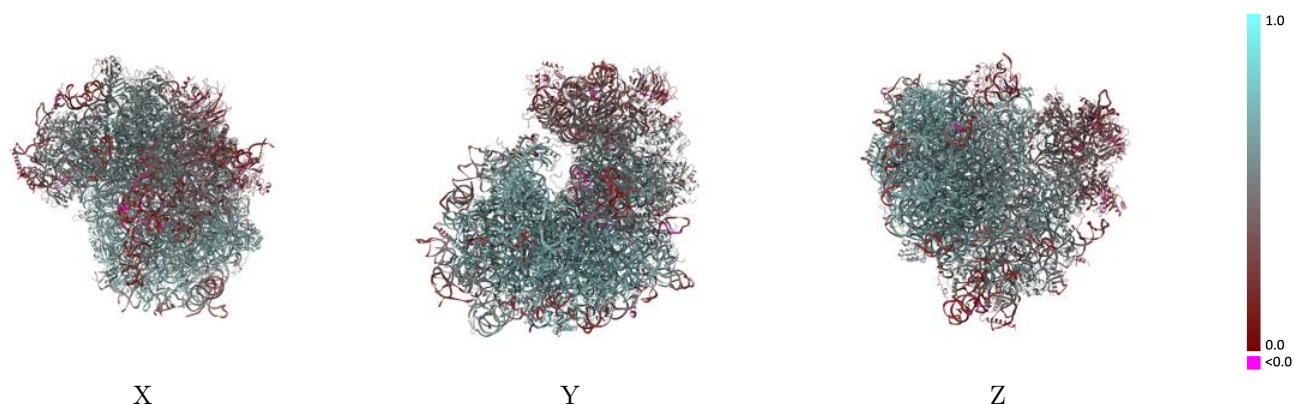
This section contains information regarding the fit between EMDB map EMD-35413 and PDB model 8IFD. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

### 9.1 Map-model overlay [i](#)



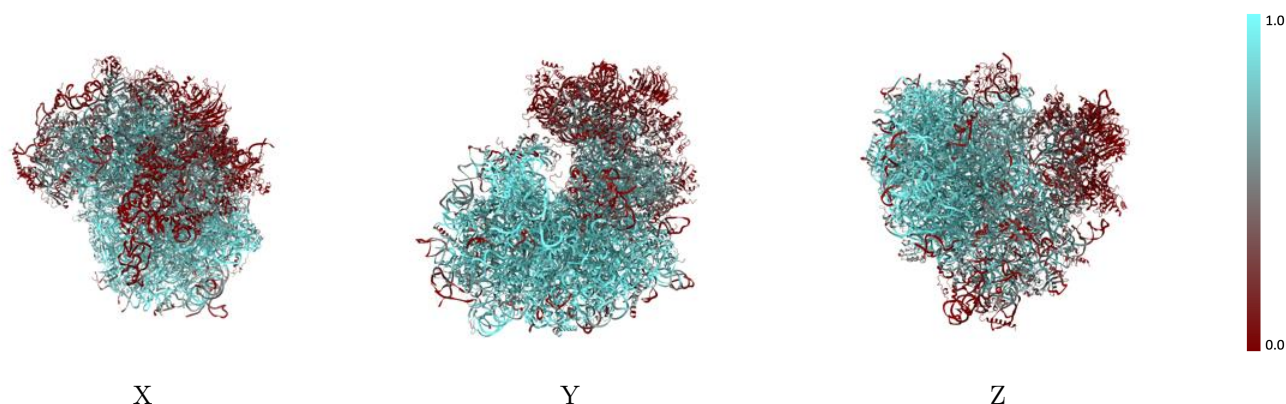
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



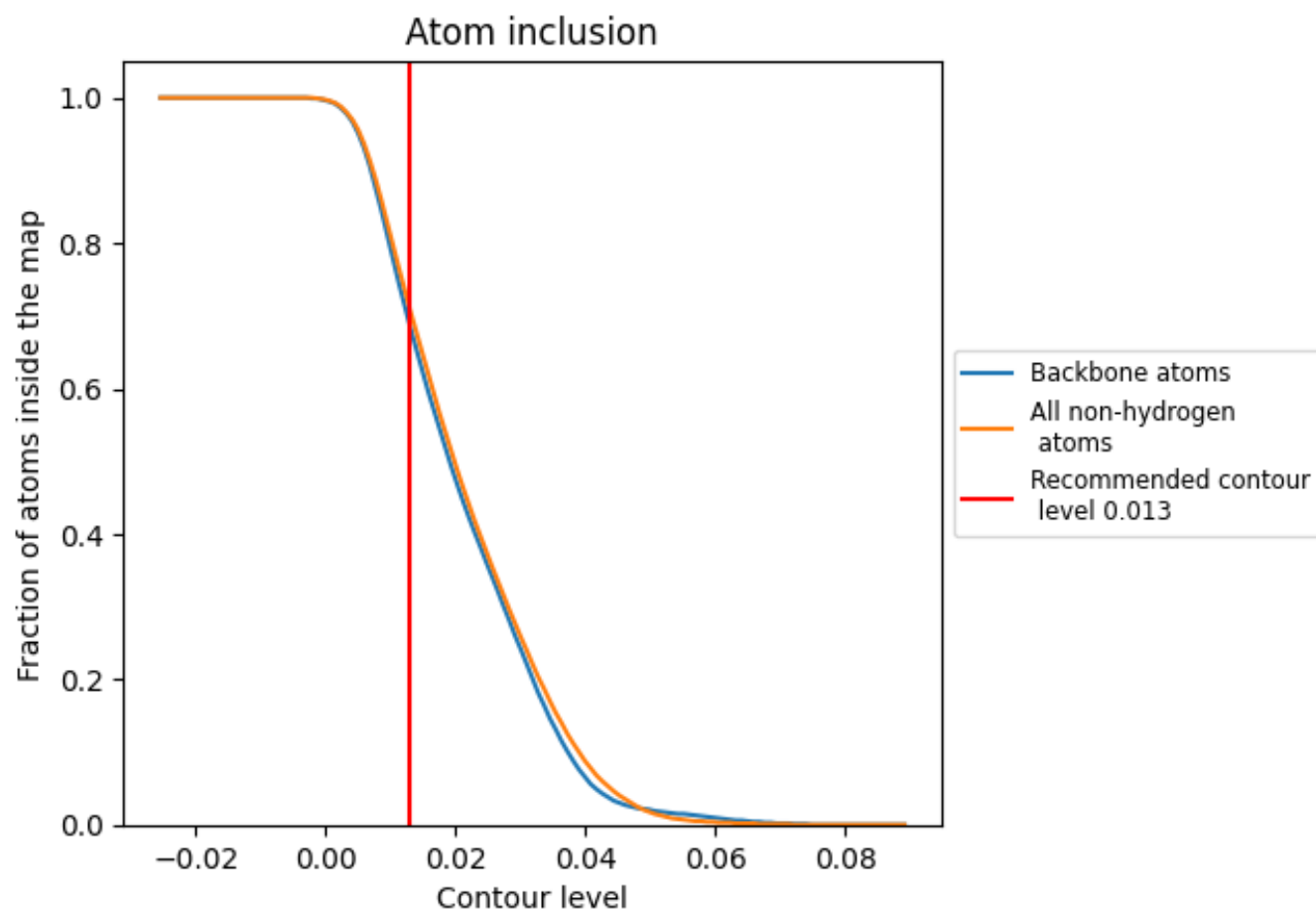
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7070   |  0.5390   |
| 1A    |  0.8460   |  0.5680   |
| 1B    |  0.9720   |  0.6270   |
| 1C    |  0.9160   |  0.6050   |
| 1D    |  0.9430   |  0.6630   |
| 1E    |  0.8880   |  0.6400   |
| 1F    |  0.8960   |  0.6400   |
| 1G    |  0.8470   |  0.6080   |
| 1H    |  0.7790   |  0.5820   |
| 20    |  0.1950   |  0.3740   |
| 21    |  0.0930   |  0.3710   |
| 2A    |  0.9050   |  0.6480   |
| 2B    |  0.7670   |  0.5710   |
| 2C    |  0.8430   |  0.6240   |
| 2D    |  0.7950  |  0.6080  |
| 2E    |  0.6190 |  0.5400 |
| 2F    |  0.8490 |  0.6090 |
| 2G    |  0.8810 |  0.6200 |
| 2H    |  0.9640 |  0.6690 |
| 2I    |  0.9020 |  0.6420 |
| 2J    |  0.9170 |  0.6590 |
| 2K    |  0.9380 |  0.6630 |
| 2L    |  0.7650 |  0.5980 |
| 2M    |  0.9190 |  0.6490 |
| 2N    |  0.8640 |  0.6350 |
| 2O    |  0.5730 |  0.5180 |
| 2P    |  0.8870 |  0.6480 |
| 2Q    |  0.4210 |  0.4260 |
| 2R    |  0.8570 |  0.6310 |
| 2S    |  0.8770 |  0.6360 |
| 2T    |  0.8580 |  0.6170 |
| 2U    |  0.9430 |  0.6620 |
| 2V    |  0.7380 |  0.5730 |
| 2W    |  0.8170 |  0.6040 |
| 2X    |  0.8550 |  0.6300 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 2Y    |  0.9230   |  0.6550   |
| 2Z    |  0.9400   |  0.6610   |
| 2a    |  0.8370   |  0.6250   |
| 2b    |  0.8650   |  0.6260   |
| 2c    |  0.8380   |  0.6180   |
| 2d    |  0.9440   |  0.6570   |
| 2e    |  0.7310   |  0.5850   |
| 2f    |  0.8860   |  0.6430   |
| 2g    |  0.8440   |  0.6350   |
| 2h    |  0.8570   |  0.6500   |
| 2i    |  0.8290   |  0.6240   |
| 2j    |  0.8680   |  0.6390   |
| 2k    |  0.9320   |  0.6430   |
| 2l    |  0.0230   |  0.2010   |
| 2m    |  0.6130   |  0.4610   |
| 2n    |  0.2280   |  0.4800   |
| 2o    |  0.5730   |  0.5480   |
| 2p    |  0.0620  |  0.3760  |
| 2q    |  0.5490 |  0.5290 |
| 2r    |  0.2010 |  0.4160 |
| 2s    |  0.2490 |  0.4530 |
| 2t    |  0.5740 |  0.5480 |
| 2u    |  0.0160 |  0.2680 |
| 2v    |  0.6040 |  0.5660 |
| 2w    |  0.0400 |  0.3410 |
| 2x    |  0.1680 |  0.3880 |
| 2y    |  0.0740 |  0.3900 |
| 2z    |  0.1530 |  0.3740 |
| 3A    |  0.3220 |  0.5070 |
| 3B    |  0.6160 |  0.5670 |
| 3C    |  0.6130 |  0.5550 |
| 3D    |  0.2080 |  0.4050 |
| 3E    |  0.2000 |  0.3870 |
| 3F    |  0.0100 |  0.2940 |
| 3G    |  0.5510 |  0.5230 |
| 3H    |  0.3120 |  0.4270 |
| 3I    |  0.4990 |  0.4940 |
| 3J    |  0.0000 |  0.1750 |
| 3K    |  0.5830 |  0.5680 |
| 3L    |  0.6190 |  0.5560 |
| 3M    |  0.6840 |  0.5720 |
| 3N    |  0.4140 |  0.4690 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| 3O    |  0.0960 |  0.3310 |
| 3P    |  0.2890 |  0.4970 |
| 3Q    |  0.3580 |  0.4730 |
| 3R    |  0.0000 |  0.1770 |