



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:04 PM UTC

PDB ID : 8OJ3 / pdb\_00008oj3  
Title : Crystal structure of the Candida albicans 80S ribosome in complex with geneticin G418 (rotated state)  
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.  
Deposited on : 2023-03-23  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

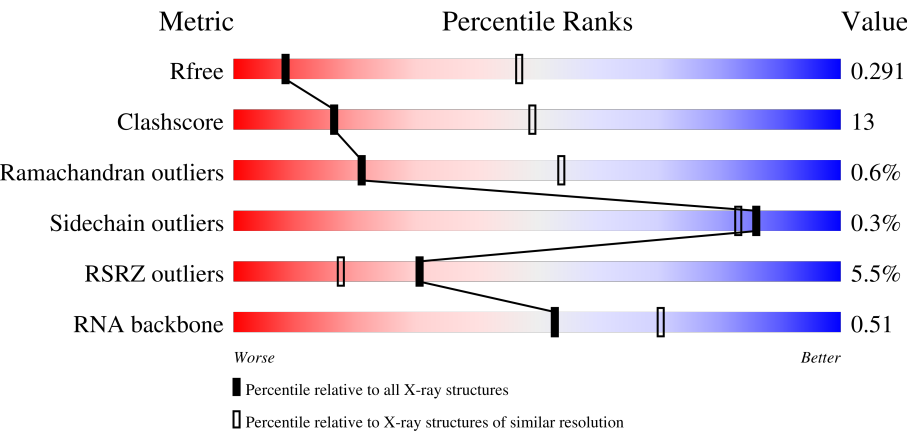
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |
| RNA backbone          | 3983                        | 1010 (3.98-3.02)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1     | 3359   |                  |
| 1   | AS    | 3359   |                  |
| 2   | 3     | 121    |                  |
| 2   | AT    | 121    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | 4     | 158    |                  |
| 3   | AU    | 158    |                  |
| 4   | AW    | 254    |                  |
| 4   | j     | 254    |                  |
| 5   | AX    | 389    |                  |
| 5   | k     | 389    |                  |
| 6   | AY    | 363    |                  |
| 6   | l     | 363    |                  |
| 7   | AZ    | 298    |                  |
| 7   | m     | 298    |                  |
| 8   | BA    | 176    |                  |
| 8   | n     | 176    |                  |
| 9   | BB    | 241    |                  |
| 9   | o     | 241    |                  |
| 10  | BC    | 262    |                  |
| 10  | p     | 262    |                  |
| 11  | BD    | 191    |                  |
| 11  | q     | 191    |                  |
| 12  | r     | 219    |                  |
| 13  | BF    | 174    |                  |
| 13  | s     | 174    |                  |
| 14  | BG    | 202    |                  |
| 14  | t     | 202    |                  |
| 15  | BH    | 131    |                  |
| 15  | u     | 131    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16  | BI    | 204    |                  |
| 16  | v     | 204    |                  |
| 17  | BJ    | 200    |                  |
| 17  | w     | 200    |                  |
| 18  | BK    | 185    |                  |
| 18  | x     | 185    |                  |
| 19  | BL    | 186    |                  |
| 19  | y     | 186    |                  |
| 20  | BM    | 190    |                  |
| 20  | z     | 190    |                  |
| 21  | 0     | 172    |                  |
| 21  | BN    | 172    |                  |
| 22  | 2     | 160    |                  |
| 22  | BO    | 160    |                  |
| 23  | 5     | 124    |                  |
| 23  | BP    | 124    |                  |
| 24  | 6     | 137    |                  |
| 24  | BQ    | 137    |                  |
| 25  | 7     | 155    |                  |
| 25  | BR    | 155    |                  |
| 26  | 8     | 142    |                  |
| 26  | BS    | 142    |                  |
| 27  | 9     | 127    |                  |
| 27  | BT    | 127    |                  |
| 28  | AA    | 136    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BU    | 136    |                  |
| 29  | AB    | 149    |                  |
| 29  | BV    | 149    |                  |
| 30  | AC    | 63     |                  |
| 30  | BW    | 63     |                  |
| 31  | AD    | 106    |                  |
| 31  | BX    | 106    |                  |
| 32  | AE    | 112    |                  |
| 32  | BY    | 112    |                  |
| 33  | AF    | 131    |                  |
| 33  | BZ    | 131    |                  |
| 34  | AG    | 107    |                  |
| 34  | CA    | 107    |                  |
| 35  | AH    | 122    |                  |
| 35  | CB    | 122    |                  |
| 36  | AI    | 120    |                  |
| 36  | CC    | 120    |                  |
| 37  | AJ    | 99     |                  |
| 37  | CD    | 99     |                  |
| 38  | AK    | 90     |                  |
| 38  | CE    | 90     |                  |
| 39  | AL    | 78     |                  |
| 39  | CF    | 78     |                  |
| 40  | AM    | 51     |                  |
| 40  | CG    | 51     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41  | AN    | 52     |                  |
| 41  | CH    | 52     |                  |
| 42  | AO    | 25     |                  |
| 42  | CI    | 25     |                  |
| 43  | AP    | 106    |                  |
| 43  | CJ    | 106    |                  |
| 44  | AQ    | 92     |                  |
| 44  | CK    | 92     |                  |
| 45  | CL    | 267    |                  |
| 45  | i     | 267    |                  |
| 46  | B     | 1787   |                  |
| 46  | CM    | 1787   |                  |
| 47  | C     | 261    |                  |
| 47  | CN    | 261    |                  |
| 48  | CO    | 256    |                  |
| 48  | D     | 256    |                  |
| 49  | CP    | 249    |                  |
| 49  | E     | 249    |                  |
| 50  | CQ    | 251    |                  |
| 50  | F     | 251    |                  |
| 51  | CR    | 262    |                  |
| 51  | G     | 262    |                  |
| 52  | CS    | 225    |                  |
| 52  | H     | 225    |                  |
| 53  | CT    | 236    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | I     | 236    |                  |
| 54  | CU    | 186    |                  |
| 54  | J     | 186    |                  |
| 55  | CV    | 206    |                  |
| 55  | K     | 206    |                  |
| 56  | CW    | 189    |                  |
| 56  | L     | 189    |                  |
| 57  | CX    | 118    |                  |
| 57  | M     | 118    |                  |
| 58  | CY    | 155    |                  |
| 58  | N     | 155    |                  |
| 59  | CZ    | 143    |                  |
| 59  | O     | 143    |                  |
| 60  | DA    | 151    |                  |
| 60  | P     | 151    |                  |
| 61  | DB    | 132    |                  |
| 61  | Q     | 132    |                  |
| 62  | DC    | 142    |                  |
| 62  | R     | 142    |                  |
| 63  | DD    | 142    |                  |
| 63  | S     | 142    |                  |
| 64  | DE    | 137    |                  |
| 64  | T     | 137    |                  |
| 65  | DF    | 145    |                  |
| 65  | U     | 145    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 66  | DG    | 145    |                  |
| 66  | V     | 145    |                  |
| 67  | DH    | 119    |                  |
| 67  | W     | 119    |                  |
| 68  | DI    | 87     |                  |
| 68  | X     | 87     |                  |
| 69  | DJ    | 130    |                  |
| 69  | Y     | 130    |                  |
| 70  | DK    | 145    |                  |
| 70  | Z     | 145    |                  |
| 71  | DL    | 135    |                  |
| 71  | a     | 135    |                  |
| 72  | DM    | 105    |                  |
| 72  | b     | 105    |                  |
| 73  | DN    | 119    |                  |
| 73  | c     | 119    |                  |
| 74  | DO    | 82     |                  |
| 74  | d     | 82     |                  |
| 75  | DP    | 67     |                  |
| 75  | e     | 67     |                  |
| 76  | DQ    | 56     |                  |
| 76  | f     | 56     |                  |
| 77  | DR    | 63     |                  |
| 77  | g     | 63     |                  |
| 78  | DS    | 193    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 78  | h     | 193    |                  |
| 79  | AR    | 317    |                  |
| 79  | DT    | 317    |                  |
| 80  | BE    | 220    |                  |
| 81  | P0    | 312    |                  |
| 82  | 12    | 165    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84  | MG   | 1     | 3508 | -         | -        | -       | X                |
| 84  | MG   | 1     | 3731 | -         | -        | -       | X                |
| 84  | MG   | 1     | 3870 | -         | -        | -       | X                |
| 84  | MG   | AS    | 3535 | -         | -        | -       | X                |
| 84  | MG   | AS    | 3641 | -         | -        | -       | X                |
| 84  | MG   | AS    | 3654 | -         | -        | -       | X                |
| 84  | MG   | CL    | 301  | -         | -        | -       | X                |

## 2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 400037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | 1     | 3218     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 68791 | 30731 | 12364 | 22478 | 3218 |         |         |       |
| 1   | AS    | 3101     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 66291 | 29614 | 11913 | 21663 | 3101 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | 3     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1153 | 463 | 842 | 121 |         |         |       |
| 2   | AT    | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1153 | 463 | 842 | 121 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 3   | 4     | 156      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3313  | 1482 | 581 | 1094 | 156 |         |         |       |
| 3   | AU    | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 585 | 1110 | 158 |         |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L2-B.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | j     | 249      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1888  | 1180 | 376 | 330 | 2 |         |         |       |
| 4   | AW    | 249      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1888  | 1180 | 376 | 330 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | k     | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3077  | 1950 | 582 | 538 | 7 |         |         |       |
| 5   | AX    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3077  | 1950 | 582 | 538 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | l     | 359      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2734  | 1720 | 524 | 487 | 3 |         |         |       |
| 6   | AY    | 359      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2734  | 1720 | 524 | 487 | 3 |         |         |       |

- Molecule 7 is a protein called Uncharacterized protein CaJ7.0206.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | m     | 294      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2409  | 1534 | 419 | 455 | 1 |         |         |       |
| 7   | AZ    | 292      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2394  | 1526 | 416 | 450 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | n     | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1242  | 796 | 226 | 219 | 1 |         |         |       |
| 8   | BA    | 153      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 1210  | 777 | 221 | 212 |   |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9   | o     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1843  | 1182 | 338 | 322 | 1 |         |         |       |
| 9   | BB    | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1816  | 1165 | 333 | 317 | 1 |         |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10  | p     | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1168 | 324 | 330 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10  | BC    | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1805  | 1156 | 321 | 325 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | q     | 190      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1519  | 958 | 276 | 281 | 4 |         |         |       |
| 11  | BD    | 190      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1519  | 958 | 276 | 281 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12  | r     | 207      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1681  | 1064 | 321 | 290 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | s     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1371  | 857 | 260 | 250 | 4 |         |         |       |
| 13  | BF    | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1371  | 857 | 260 | 250 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 14  | t     | 200      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1610  | 1009 | 318 | 283 |         |         |       |
| 14  | BG    | 200      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1610  | 1009 | 318 | 283 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | u     | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1015  | 651 | 190 | 173 | 1 |         |         |       |
| 15  | BH    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1029  | 660 | 193 | 175 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 16  | v     | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1713  | 1075 | 356 | 280 | 2 |         |         |       |
| 16  | BI    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1713  | 1075 | 356 | 280 | 2 |         |         |       |

- Molecule 17 is a protein called Ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 17  | w     | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 1025 | 294 | 269 | 2 |         |         |       |
| 17  | BJ    | 199      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1590  | 1025 | 294 | 269 | 2 |         |         |       |

- Molecule 18 is a protein called Ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18  | x     | 169      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1352  | 835 | 273 | 244 |         |         |       |
| 18  | BK    | 174      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1396  | 862 | 282 | 252 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19  | y     | 185      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1458  | 916 | 297 | 245 |         |         |       |
| 19  | BL    | 185      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1458  | 916 | 297 | 245 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | z     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1457  | 901 | 310 | 243 | 3 |         |         |       |
| 20  | BM    | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1457  | 901 | 310 | 243 | 3 |         |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | 0     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1423  | 921 | 258 | 241 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | BN    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1423  | 921 | 258 | 241 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 2     | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1262  | 798 | 241 | 221 | 2 |         |         |       |
| 22  | BO    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1262  | 798 | 241 | 221 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | 5     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 803   | 518 | 135 | 150 |   |         |         |       |
| 23  | BP    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 512 | 133 | 149 |   |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | 6     | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 615 | 183 | 171 | 8 |         |         |       |
| 24  | BQ    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 615 | 183 | 171 | 8 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | 7     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 945   | 591 | 192 | 161 | 1 |         |         |       |
| 25  | BR    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 549 | 178 | 149 | 1 |         |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | 8     | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 616 | 173 | 175 | 1 |         |         |       |
| 26  | BS    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 960   | 613 | 172 | 174 | 1 |         |         |       |

- Molecule 27 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 27  | 9     | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 989   | 618 | 190 | 181 |         |         |       |
| 27  | BT    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 989   | 618 | 190 | 181 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | AA    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1087  | 705 | 197 | 183 | 2 |         |         |       |
| 28  | BU    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1087  | 705 | 197 | 183 | 2 |         |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | AB    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1170  | 741 | 231 | 197 | 1 |         |         |       |
| 29  | BV    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1170  | 741 | 231 | 197 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 30  | AC    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 464   | 290 | 100 | 74 |         |         |       |
| 30  | BW    | 60       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 482   | 301 | 103 | 78 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | AD    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 747   | 479 | 124 | 142 | 2 |         |         |       |
| 31  | BX    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 715   | 460 | 119 | 134 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | AE    | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 881   | 556 | 166 | 157 | 2 |         |         |       |
| 32  | BY    | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 881   | 556 | 166 | 157 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | AF    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1000  | 638 | 194 | 167 | 1 |         |         |       |
| 33  | BZ    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 991   | 633 | 192 | 165 | 1 |         |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | AG    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 543 | 161 | 142 | 1 |         |         |       |
| 34  | CA    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 543 | 161 | 142 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | AH    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 887   | 547 | 182 | 154 | 4 |         |         |       |
| 35  | CB    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 869   | 536 | 179 | 150 | 4 |         |         |       |

- Molecule 36 is a protein called Ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 36  | AI    | 115      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 963   | 611 | 190 | 162 |  |         |         |       |
| 36  | CC    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 974   | 618 | 192 | 164 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | AJ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 758   | 471 | 156 | 130 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | CD    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 736   | 459 | 148 | 128 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | AK    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 677   | 413 | 148 | 110 | 6 |         |         |       |
| 38  | CE    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 677   | 413 | 148 | 110 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 39  | AL    | 77       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 617   | 393 | 115 | 109 |  |         |         |       |
| 39  | CF    | 77       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 617   | 393 | 115 | 109 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 40  | AM    | 50       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 438   | 275 | 97 | 66 |  |         |         |       |
| 40  | CG    | 50       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 438   | 275 | 97 | 66 |  |         |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L40-B.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 41  | AN    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 402   | 249 | 83 | 65 | 5 |         |         |       |
| 41  | CH    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 249 | 84 | 65 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 42  | AO    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 236   | 144 | 63 | 28 | 1 |         |         |       |
| 42  | CI    | 24       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 227   | 138 | 61 | 27 | 1 |         |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L42-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | AP    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 828   | 521 | 165 | 137 | 5 |         |         |       |
| 43  | CJ    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 828   | 521 | 165 | 137 | 5 |         |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | AQ    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 698   | 430 | 140 | 124 | 4 |         |         |       |
| 44  | CK    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 698   | 430 | 140 | 124 | 4 |         |         |       |

- Molecule 45 is a protein called 60S ribosomal protein CAALFM\_C304810CA.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 45  | i     | 106      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 805   | 483 | 147 | 175 |  |         |         |       |
| 45  | CL    | 120      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 919   | 554 | 165 | 200 |  |         |         |       |

- Molecule 46 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 46  | B     | 1708     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 36410 | 16276 | 6460 | 11966 | 1708 |         |         |       |
| 46  | CM    | 1728     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 36839 | 16468 | 6538 | 12105 | 1728 |         |         |       |

- Molecule 47 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 47  | C     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1041 | 284 | 297 | 5 |         |         |       |
| 47  | CN    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1041 | 284 | 297 | 5 |         |         |       |

- Molecule 48 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 48  | D     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1724  | 1094 | 313 | 313 | 4 |         |         |       |
| 48  | CO    | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1717  | 1089 | 312 | 312 | 4 |         |         |       |

- Molecule 49 is a protein called Ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 49  | E     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1629  | 1039 | 289 | 296 | 5 |         |         |       |
| 49  | CP    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1629  | 1039 | 289 | 296 | 5 |         |         |       |

- Molecule 50 is a protein called Ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 50  | F     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1707  | 1087 | 311 | 305 | 4 |         |         |       |
| 50  | CQ    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1707  | 1087 | 311 | 305 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51  | G     | 258      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2042  | 1299 | 383 | 355 | 5 |         |         |       |
| 51  | CR    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2055  | 1306 | 386 | 358 | 5 |         |         |       |

- Molecule 52 is a protein called Ribosomal protein S7.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | H     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1614  | 1008 | 301 | 301 | 4 |         |         |       |
| 52  | CS    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1606  | 1002 | 300 | 300 | 4 |         |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 53  | I     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1798  | 1119 | 348 | 325 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 53  | CT    | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1904  | 1184 | 369 | 345 | 6 |         |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | J     | 182      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1466  | 939 | 264 | 263 |   |         |         |       |
| 54  | CU    | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1449  | 929 | 261 | 259 |   |         |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | K     | 203      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1579  | 973 | 322 | 283 | 1 |         |         |       |
| 55  | CV    | 203      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1579  | 973 | 322 | 283 | 1 |         |         |       |

- Molecule 56 is a protein called Ribosomal protein S4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | L     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1453  | 918 | 286 | 248 | 1 |         |         |       |
| 56  | CW    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1453  | 918 | 286 | 248 | 1 |         |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | M     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 817   | 531 | 135 | 150 | 1 |         |         |       |
| 57  | CX    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 791   | 515 | 131 | 144 | 1 |         |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S11A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58  | N     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1150  | 734 | 215 | 198 | 3 |         |         |       |
| 58  | CY    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 722 | 212 | 192 | 3 |         |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59  | O     | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 550 | 158 | 172 | 5 |         |         |       |
| 59  | CZ    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 913   | 566 | 163 | 179 | 5 |         |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60  | P     | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1175  | 749 | 217 | 208 | 1 |         |         |       |
| 60  | DA    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1187  | 757 | 219 | 210 | 1 |         |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61  | Q     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 942   | 579 | 186 | 174 | 3 |         |         |       |
| 61  | DB    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 905   | 555 | 180 | 167 | 3 |         |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 62  | R     | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1034  | 658 | 190 | 179 | 7 |         |         |       |
| 62  | DC    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1029  | 655 | 189 | 178 | 7 |         |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 63  | S     | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1085  | 697 | 197 | 190 | 1 |         |         |       |
| 63  | DD    | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1085  | 697 | 197 | 190 | 1 |         |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64  | T     | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 628 | 183 | 185 | 1 |         |         |       |
| 64  | DE    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 628 | 183 | 185 | 1 |         |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 65  | U     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1187  | 744 | 233 | 207 | 3 |         |         |       |
| 65  | DF    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1161  | 727 | 227 | 204 | 3 |         |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 66  | V     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1100  | 689 | 210 | 200 | 1 |         |         |       |
| 66  | DG    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1100  | 689 | 210 | 200 | 1 |         |         |       |

- Molecule 67 is a protein called Ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 67  | W     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 808   | 509 | 150 | 147 | 2 |         |         |       |
| 67  | DH    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 140 | 140 | 2 |         |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | X     | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 415 | 126 | 133 | 2 |         |         |       |
| 68  | DI    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 415 | 126 | 133 | 2 |         |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69  | Y     | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 655 | 191 | 183 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69  | DJ    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 655 | 191 | 183 | 3 |         |         |       |

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 70  | Z     | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 701 | 219 | 188 | 2 |         |         |       |
| 70  | DK    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 701 | 219 | 188 | 2 |         |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 71  | a     | 134      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1086  | 677 | 218 | 191 |  |         |         |       |
| 71  | DL    | 132      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1072  | 670 | 216 | 186 |  |         |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 72  | b     | 72       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 578   | 369 | 103 | 106 |  |         |         |       |
| 72  | DM    | 71       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 570   | 365 | 102 | 103 |  |         |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73  | c     | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 477 | 161 | 126 | 6 |         |         |       |
| 73  | DN    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 482 | 163 | 128 | 6 |         |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 74  | d     | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 614   | 383 | 110 | 114 | 7 |         |         |       |
| 74  | DO    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 614   | 383 | 110 | 114 | 7 |         |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 75  | e     | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 468   | 287 | 93 | 86 | 2 |         |         |       |
| 75  | DP    | 61       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 476   | 293 | 94 | 87 | 2 |         |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S29A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 76  | f     | 55       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 454   | 281 | 94 | 75 | 4 |         |         |       |
| 76  | DQ    | 54       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 278 | 93 | 74 | 4 |         |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 77  | g     | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 474   | 297 | 96 | 79 | 2 |         |         |       |
| 77  | DR    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 470   | 295 | 95 | 78 | 2 |         |         |       |

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 78  | h     | 70       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 574   | 362 | 113 | 93 | 6 |         |         |       |
| 78  | DS    | 68       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 555   | 350 | 108 | 91 | 6 |         |         |       |

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 79  | AR    | 311      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2398  | 1519 | 412 | 462 | 5 |         |         |       |
| 79  | DT    | 307      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2362  | 1498 | 403 | 456 | 5 |         |         |       |

- Molecule 80 is a protein called 60S ribosomal protein L10.



| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 80  | BE    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1662  | 1052 | 318 | 285 | 7 |         |         |       |

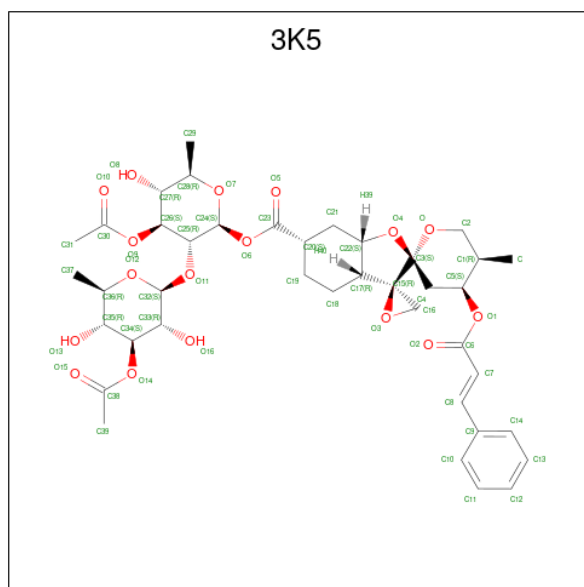
- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 81  | P0    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 845   | 542 | 150 | 150 | 3 |         |         |       |

- Molecule 82 is a protein called 60S ribosomal protein L12-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 82  | 12    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 480   | 297 | 85 | 96 | 2 |         |         |       |

- Molecule 83 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (CCD ID: 3K5) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>17</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 83  | 1     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 57    | 40 | 17 |         |         |
| 83  | AS    | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 57    | 40 | 17 |         |         |

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 84  | 1     | 469      | Total Mg<br>469 469 | 0       | 0       |
| 84  | 3     | 7        | Total Mg<br>7 7     | 0       | 0       |
| 84  | 4     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | j     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | k     | 3        | Total Mg<br>3 3     | 0       | 0       |
| 84  | m     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | o     | 4        | Total Mg<br>4 4     | 0       | 0       |
| 84  | r     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | u     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | v     | 2        | Total Mg<br>2 2     | 0       | 0       |
| 84  | w     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | x     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | y     | 3        | Total Mg<br>3 3     | 0       | 0       |
| 84  | 0     | 4        | Total Mg<br>4 4     | 0       | 0       |
| 84  | 2     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | 6     | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | AB    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 84  | AC    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | AD    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | AJ    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 84  | AP    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 84  | B     | 99       | Total Mg<br>99 99   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 84  | C     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | D     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | E     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | F     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | G     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | K     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | L     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | Q     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 84  | R     | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 84  | T     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | Y     | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 84  | a     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | AS    | 389      | Total<br>389 | Mg<br>389 | 0       | 0       |
| 84  | AT    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 84  | AU    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 84  | AW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | AX    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 84  | AY    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 84  | AZ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 84  | BB    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 84  | BC    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 84  | BE    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | BI    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | BK    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | BL    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 84  | BO    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | BQ    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | BZ    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | CA    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | CB    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | CG    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | CL    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 84  | CM    | 78       | Total<br>78 | Mg<br>78 | 0       | 0       |
| 84  | CW    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | DA    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | DG    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | DH    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 84  | DK    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 84  | P0    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

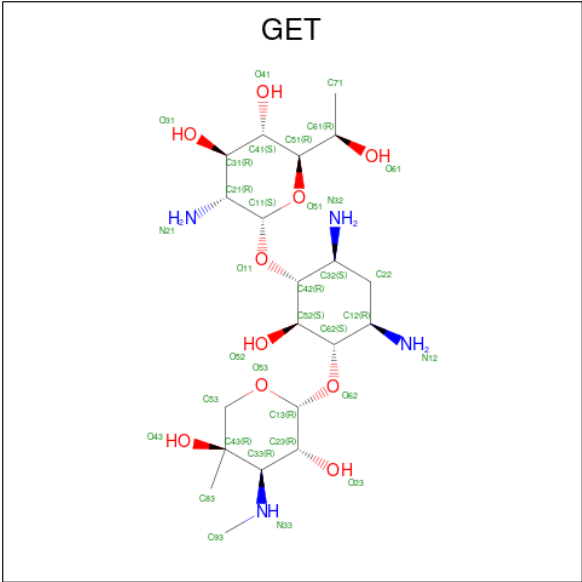
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 85  | AH    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 85  | AK    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | AN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | AP    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | AQ    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | c     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | d     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | f     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | h     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | CB    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | CE    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | CH    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | CJ    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | CK    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | DN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | DQ    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 85  | DS    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 86 is GENETICIN (CCD ID: GET) (formula:  $C_{20}H_{40}N_4O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



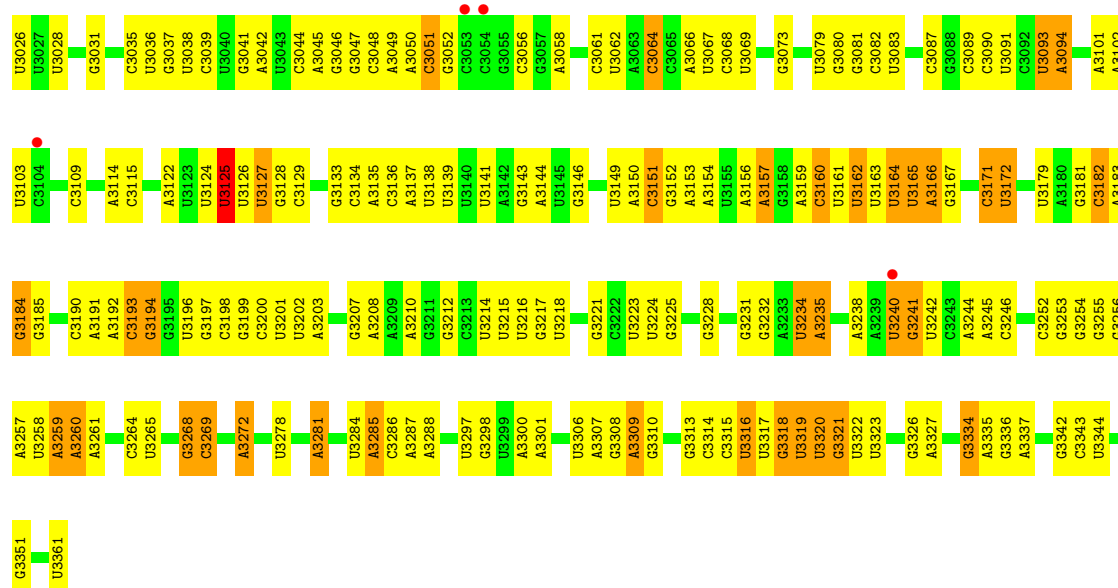
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 86  | B     | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |         |
| 86  | CM    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |         |



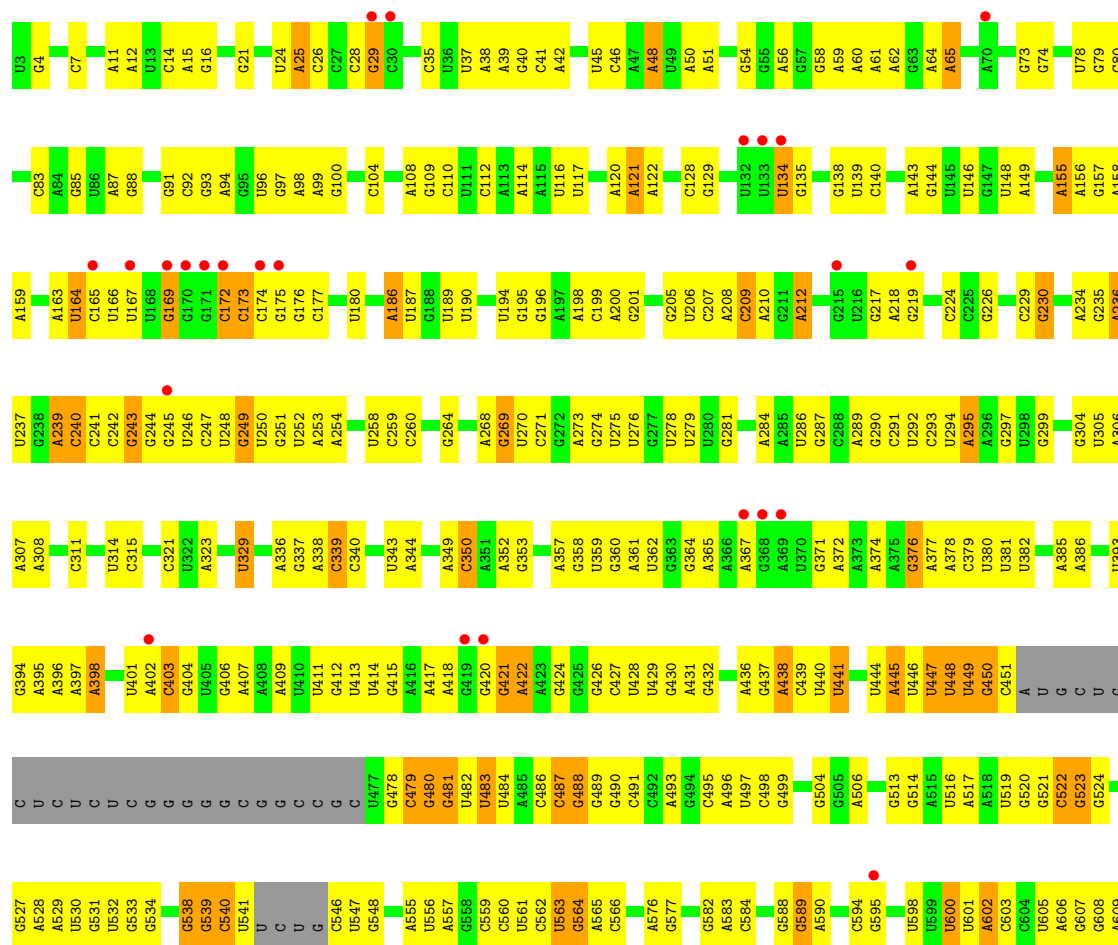
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1808 | A1809 | A1810 | U1811 | A1812 | G1813 | U1814 | U1815 | U1816 | G1817 | A1825 | G1826 | A1831 | A1832 | A1833 | A1834 | A1835 | U1836 | A1837 | A1838 | G1841 | G1842 | C1845 | A1851 | C1852 | C1853 | G1857 | U1858 | A1859 | A1860 | A1861 | C1862 | A1863 | A1864 | A1865 | C1866 | U1867 | G1874 | U1791 | G1792 | A1793 | A1794 | A1795 | C1796 | C1799 | A1800 | A1892 | G1893 | G1894 | G1895 | C1900 | G1901 |       |       |       |       |       |
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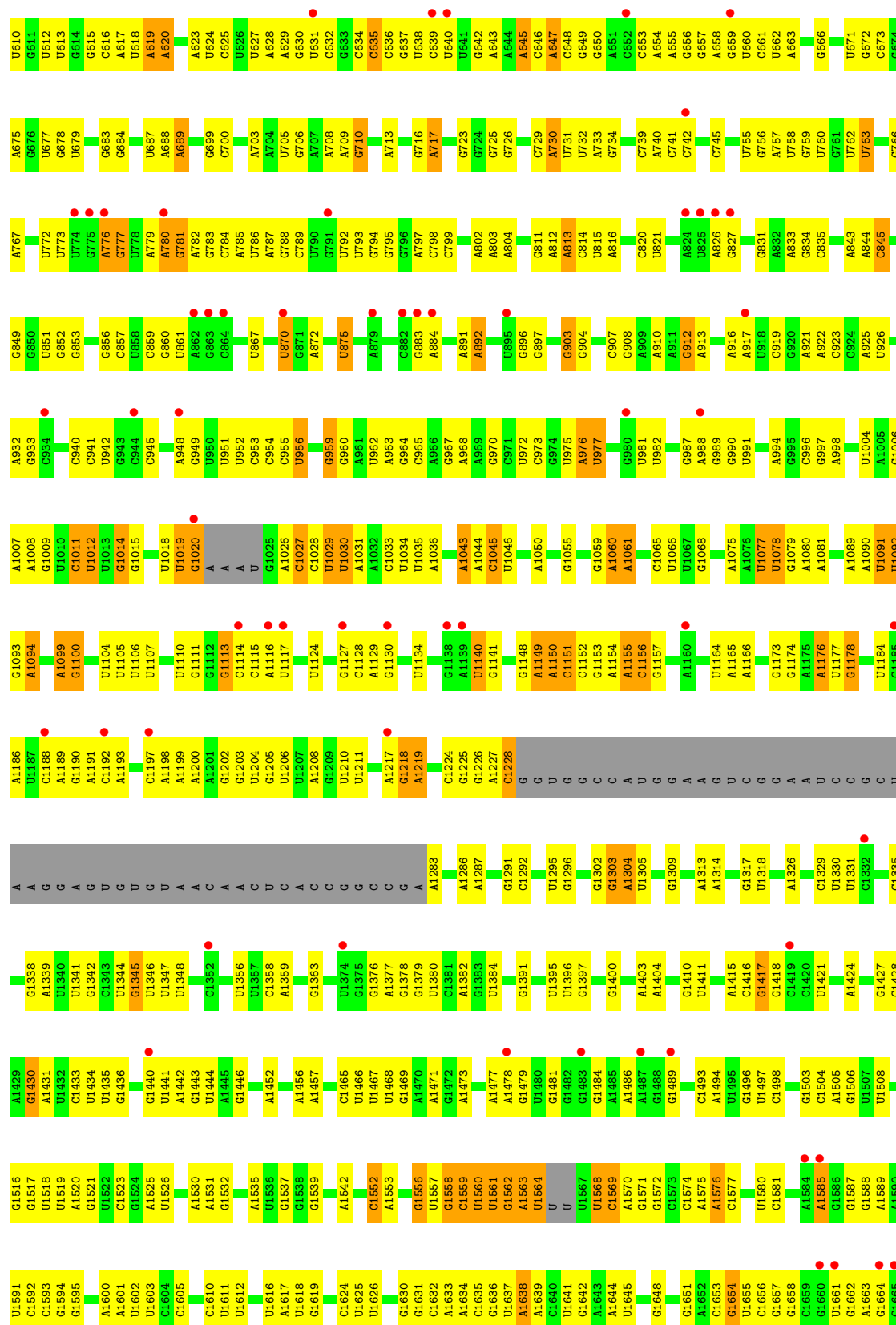


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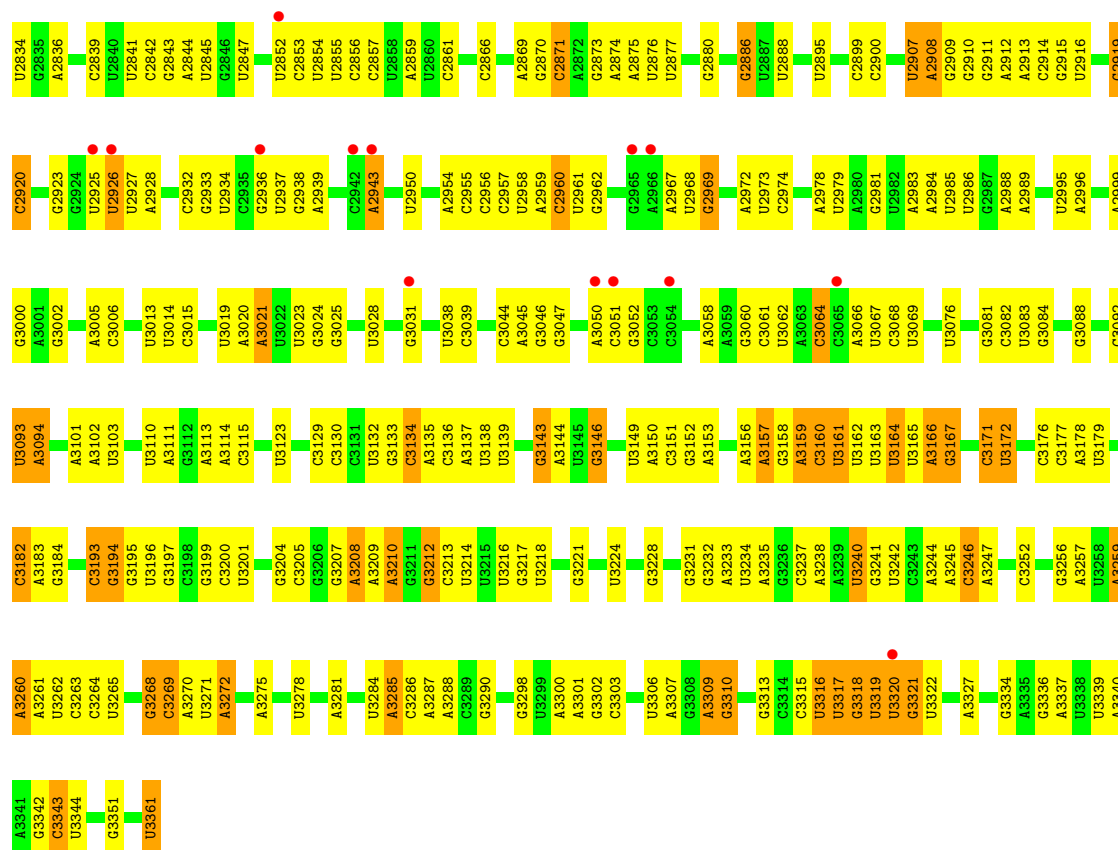


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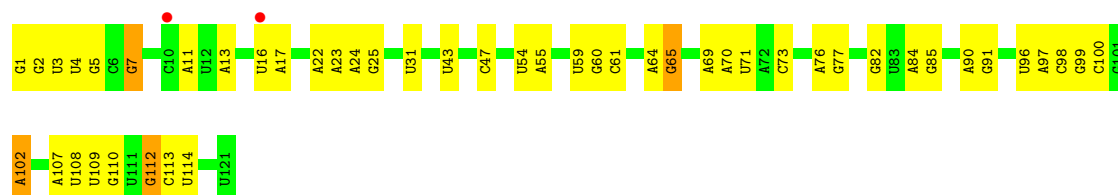




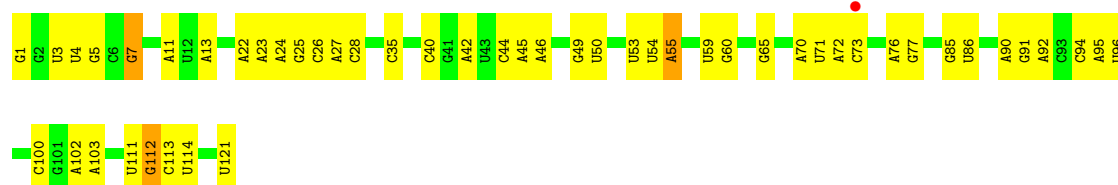




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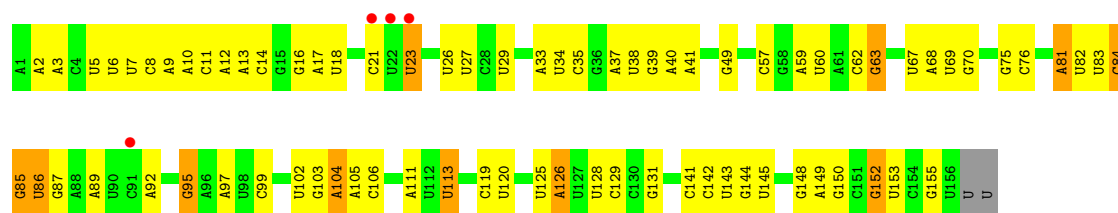


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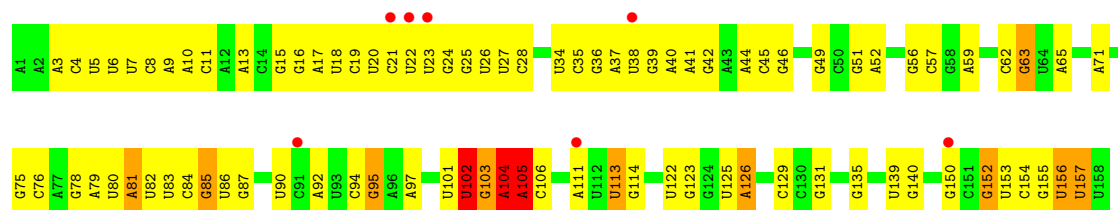


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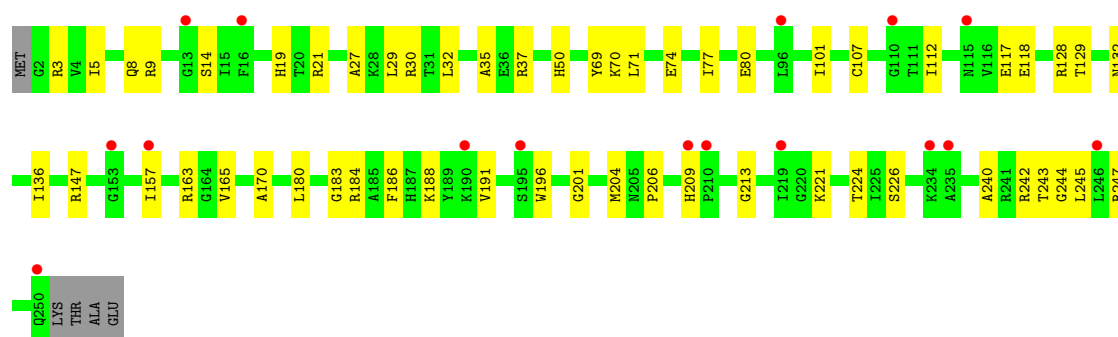
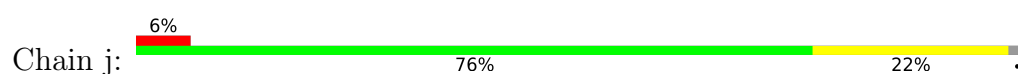




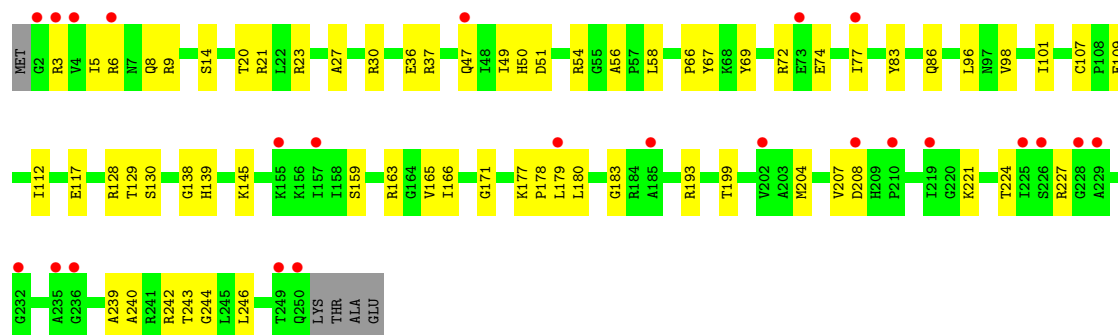
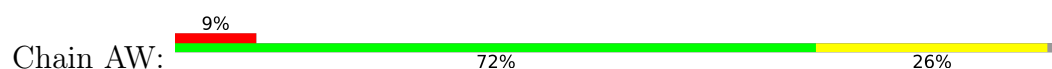
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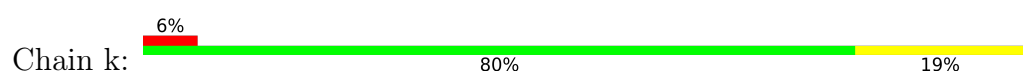
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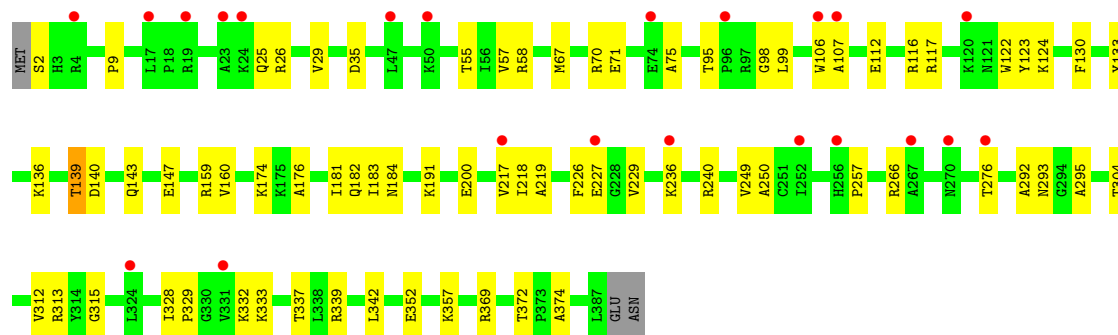


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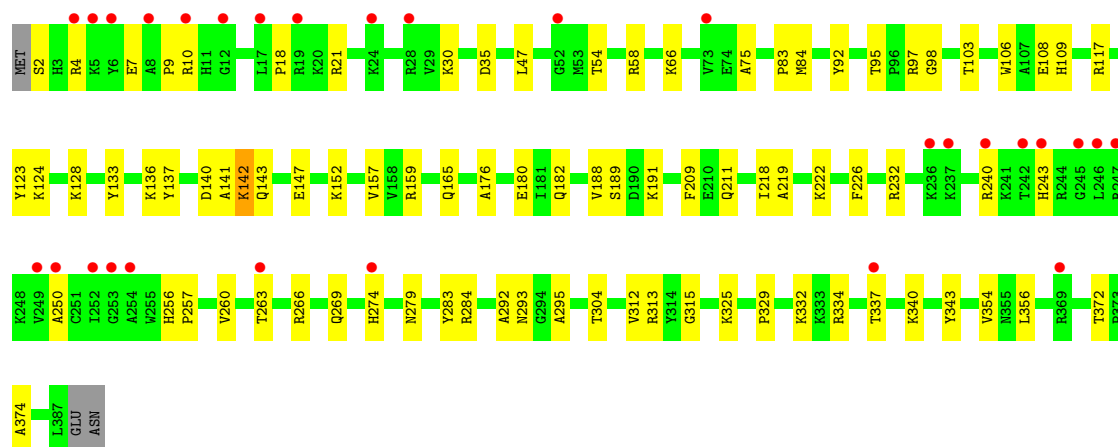
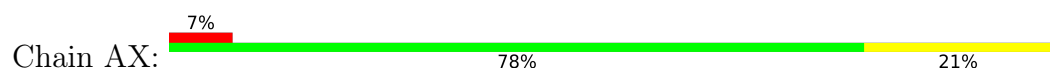


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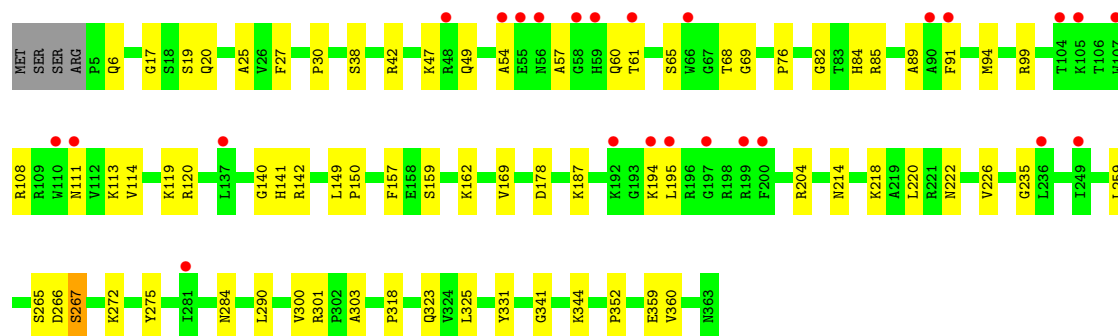
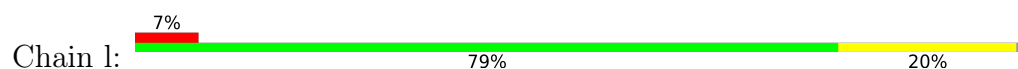




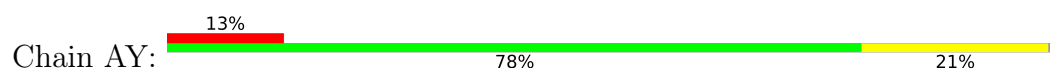
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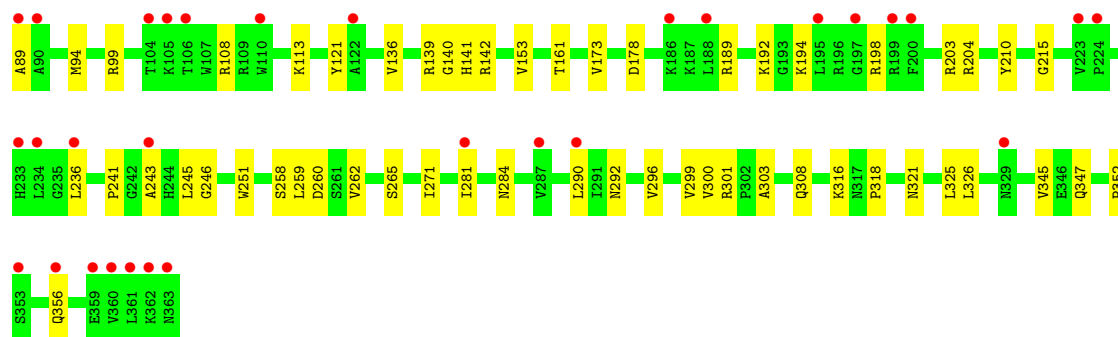


• Molecule 6: 60S ribosomal protein L4-B

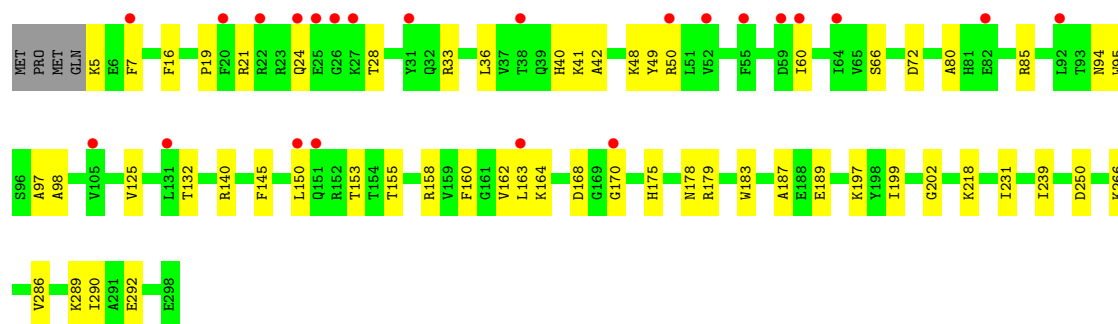
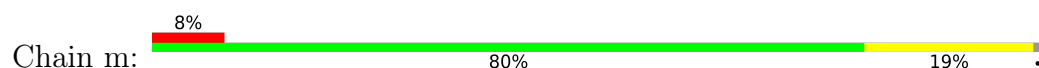


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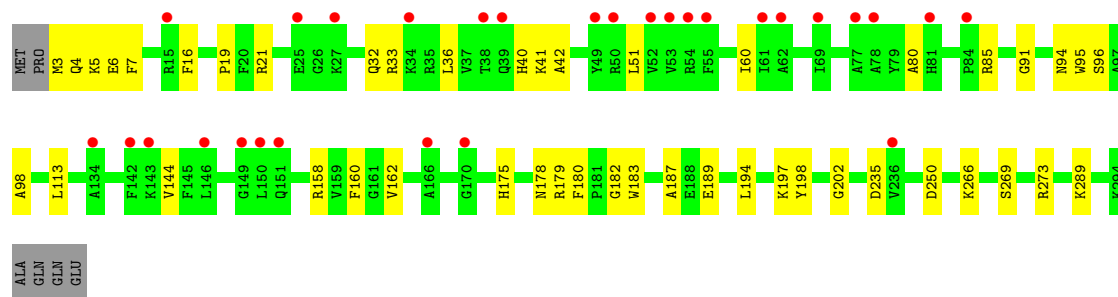
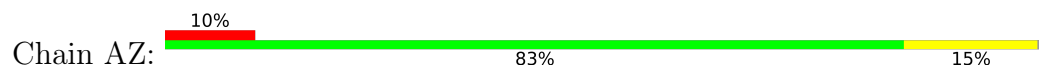




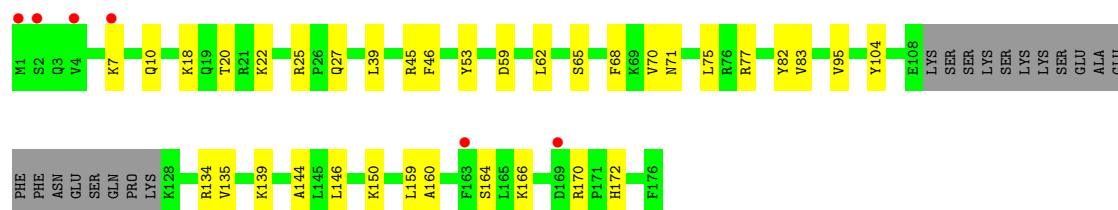
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• Molecule 7: Uncharacterized protein CaJ7.0206



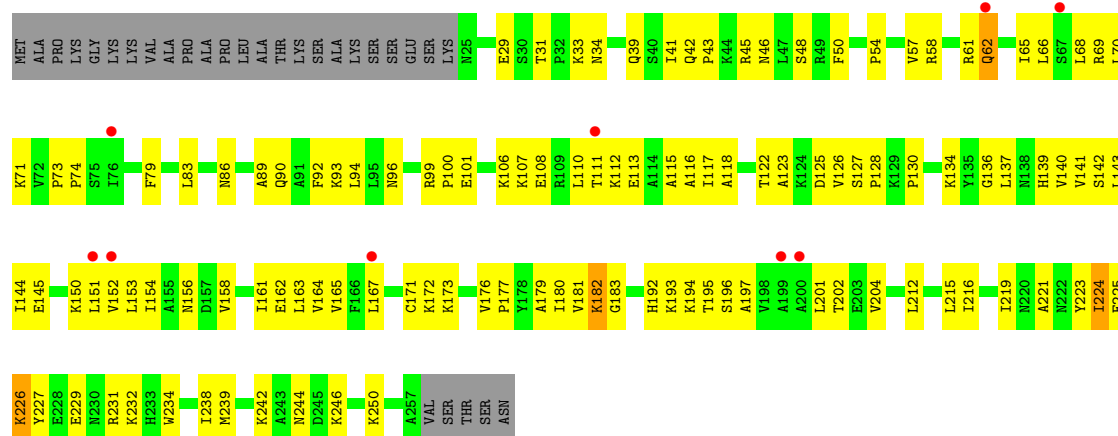
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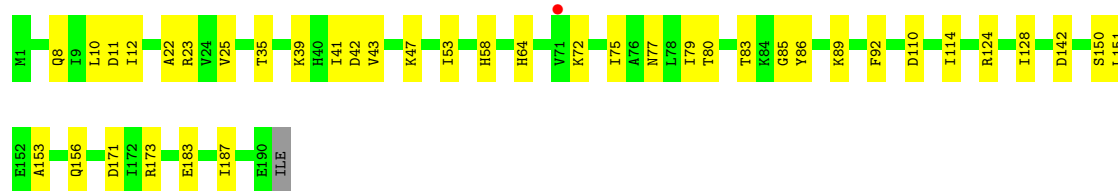
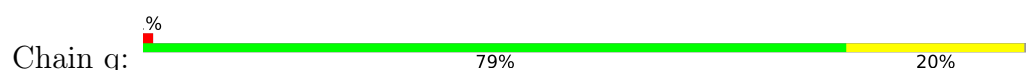
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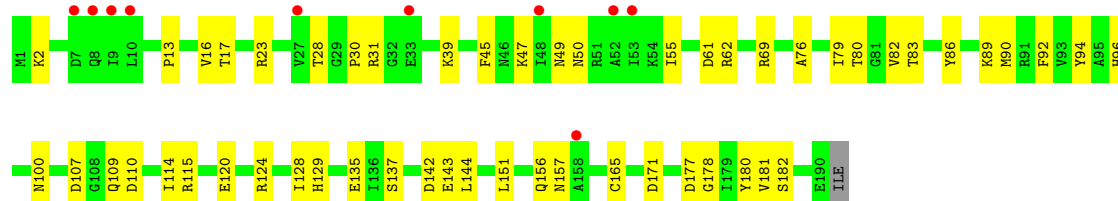
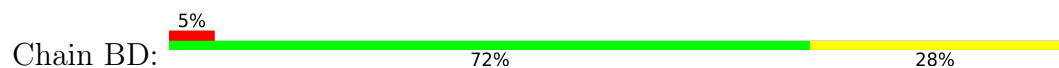




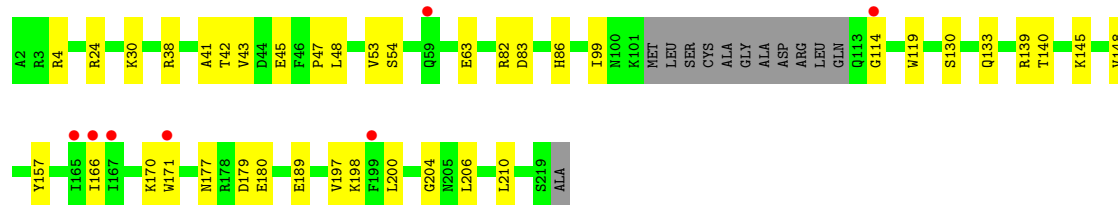
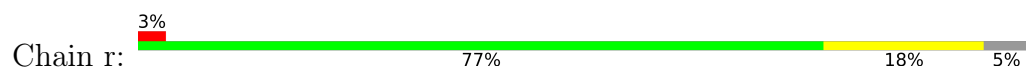
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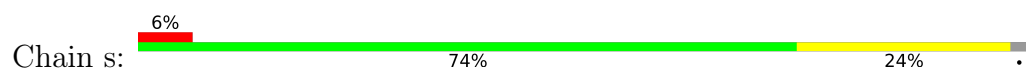
• Molecule 11: 60S ribosomal protein L9-B

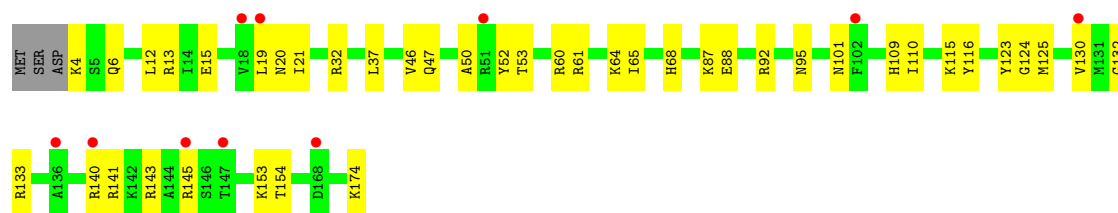


• Molecule 12: 60S ribosomal protein L10

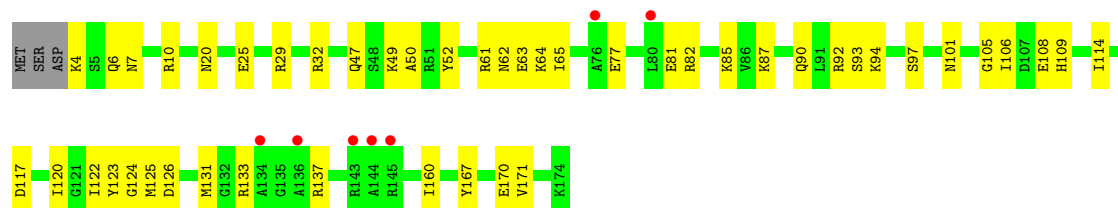
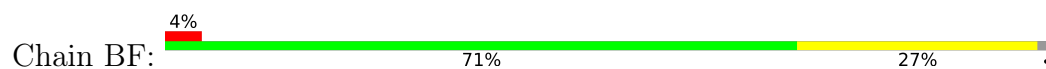


• Molecule 13: 60S ribosomal protein L11-B

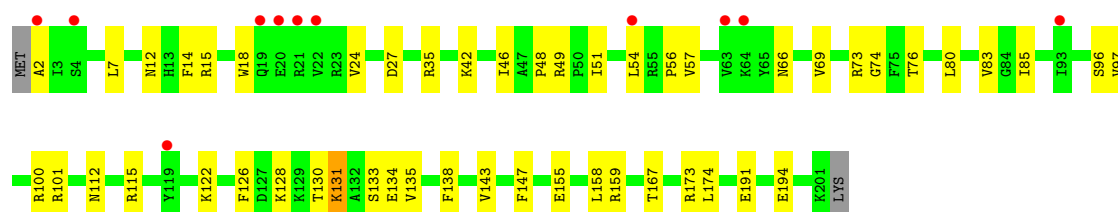
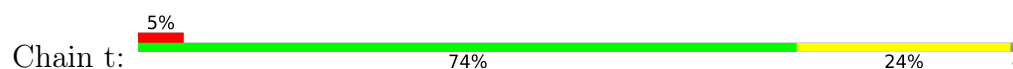




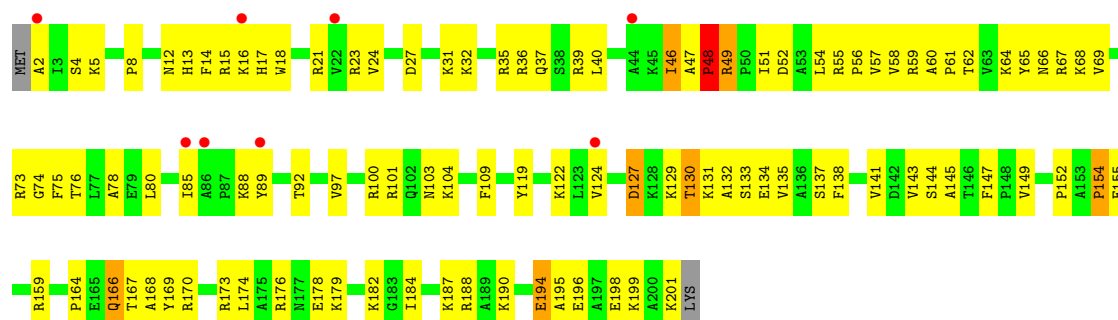
• Molecule 13: 60S ribosomal protein L11-B



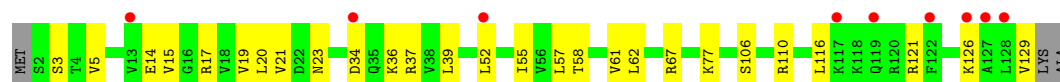
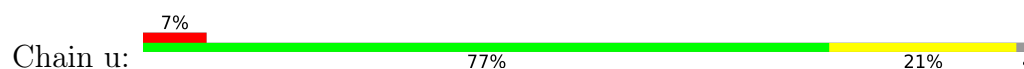
• Molecule 14: 60S ribosomal protein L13



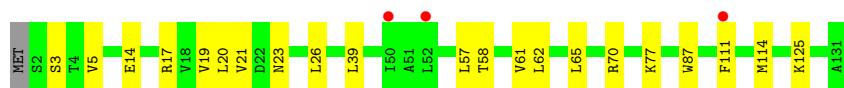
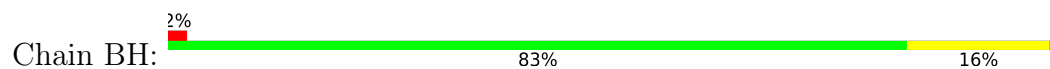
• Molecule 14: 60S ribosomal protein L13



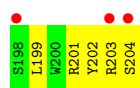
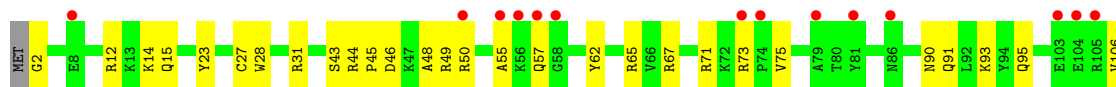
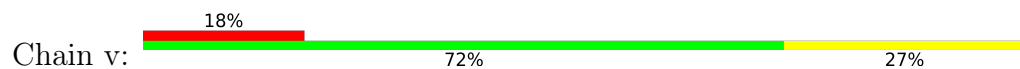
• Molecule 15: 60S ribosomal protein L14-B



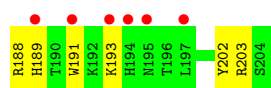
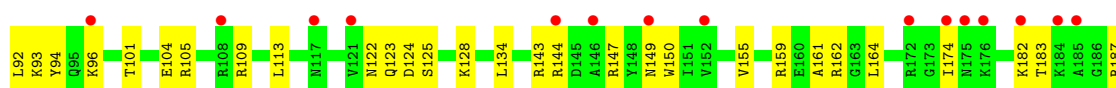
- Molecule 15: 60S ribosomal protein L14-B



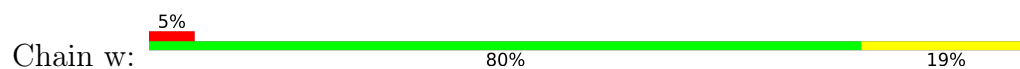
- Molecule 16: 60S ribosomal protein L15-A



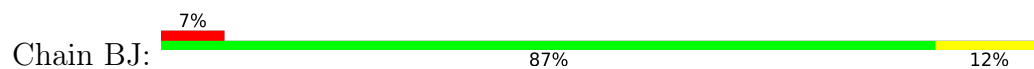
- Molecule 16: 60S ribosomal protein L15-A

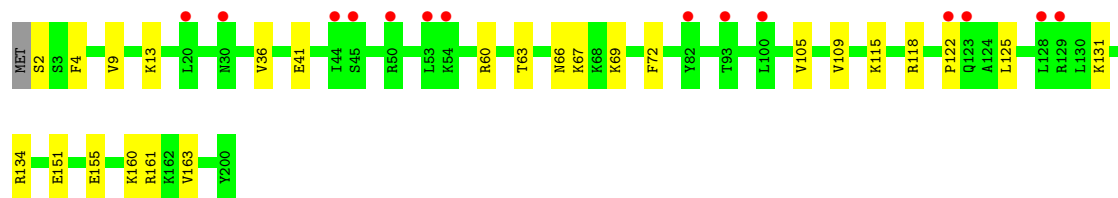


- Molecule 17: Ribosomal protein L13

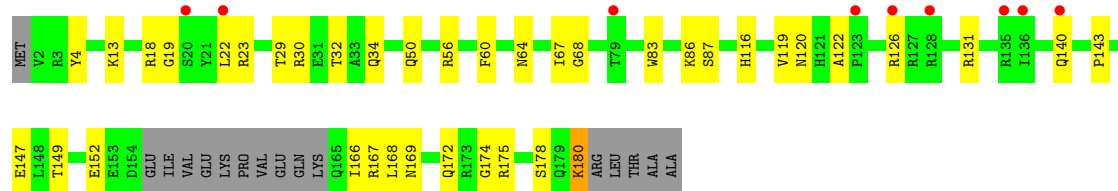


- Molecule 17: Ribosomal protein L13

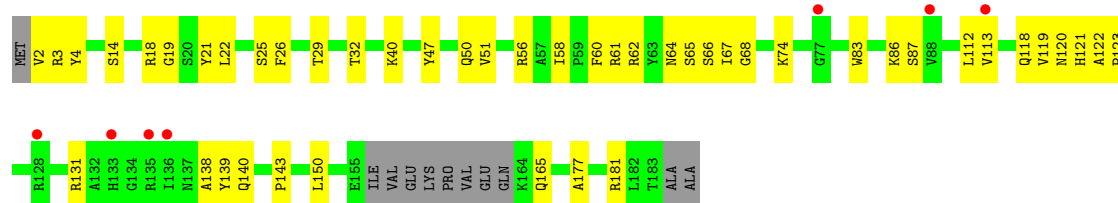




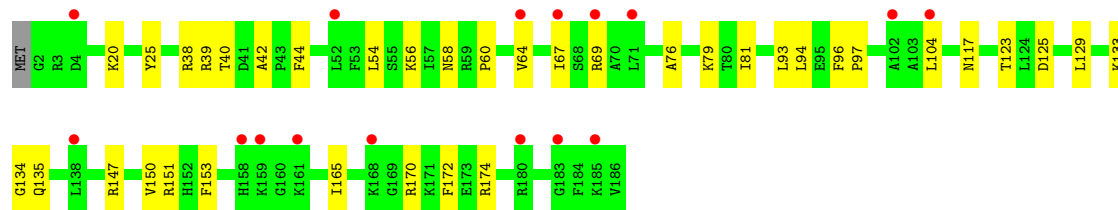
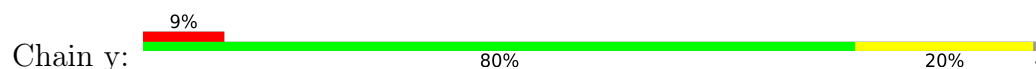
• Molecule 18: Ribosomal protein L22



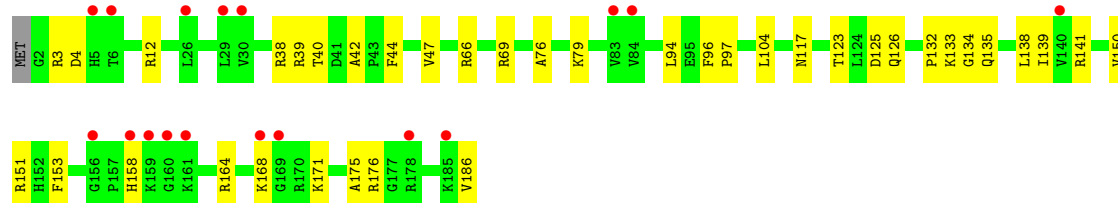
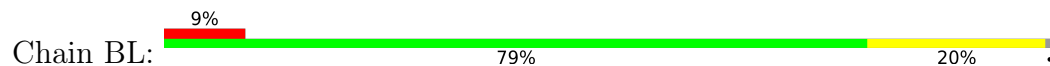
• Molecule 18: Ribosomal protein L22



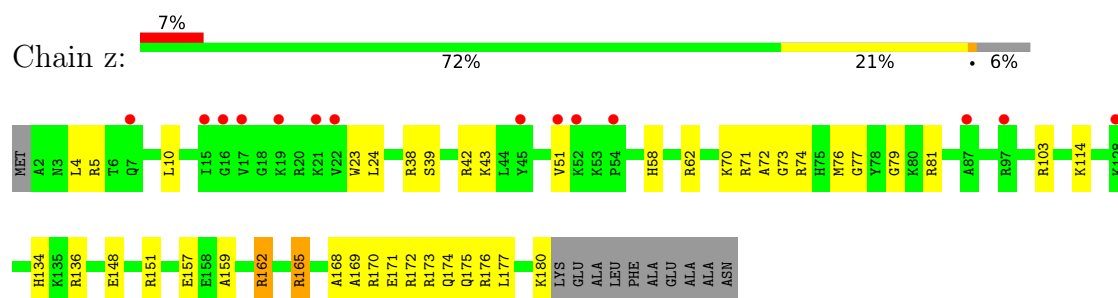
• Molecule 19: 60S ribosomal protein L18-A



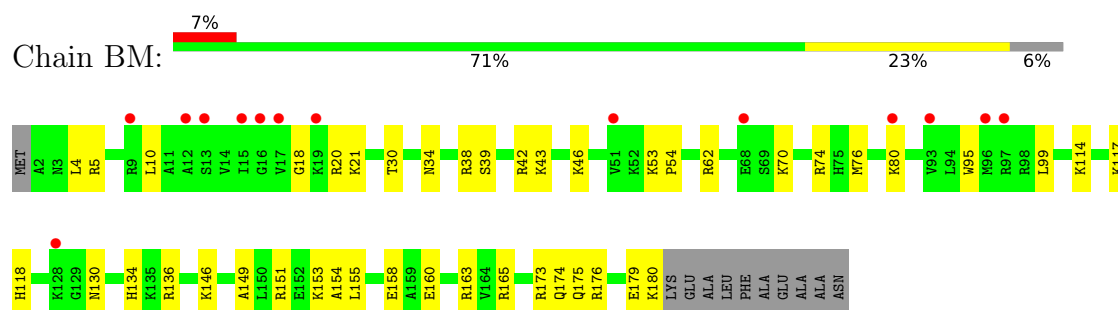
• Molecule 19: 60S ribosomal protein L18-A



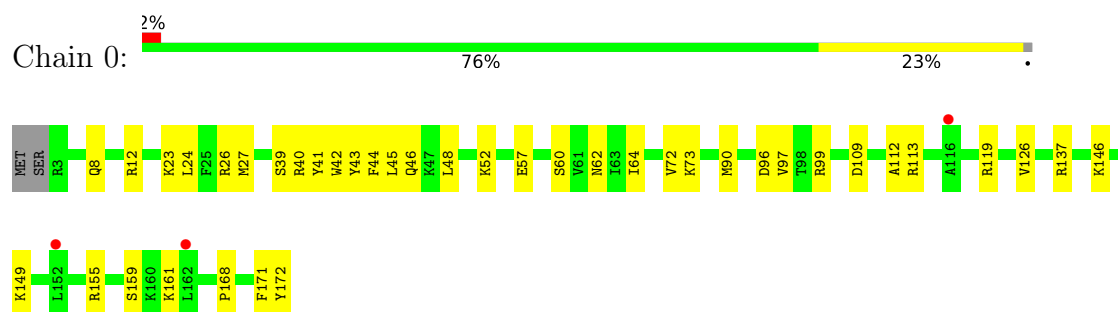
- Molecule 20: 60S ribosomal protein L19-A



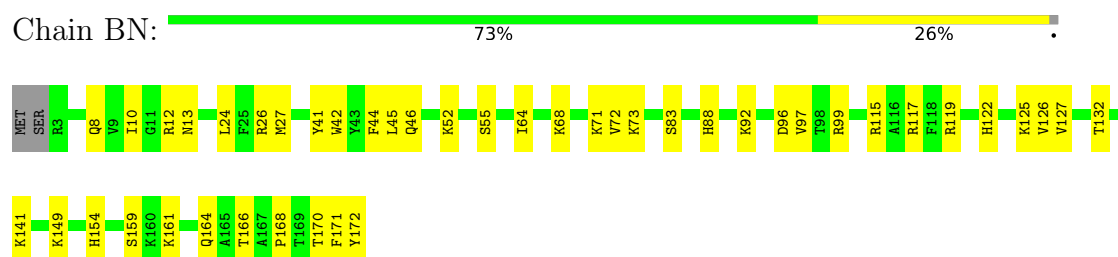
- Molecule 20: 60S ribosomal protein L19-A



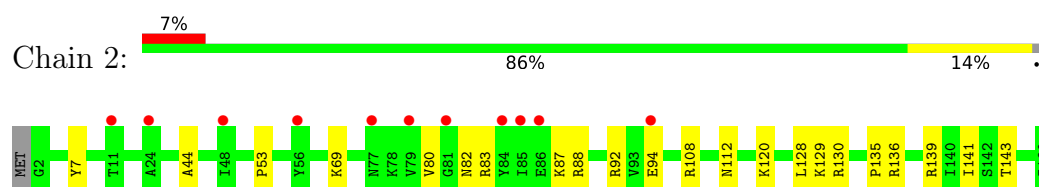
- Molecule 21: 60S ribosomal protein L20



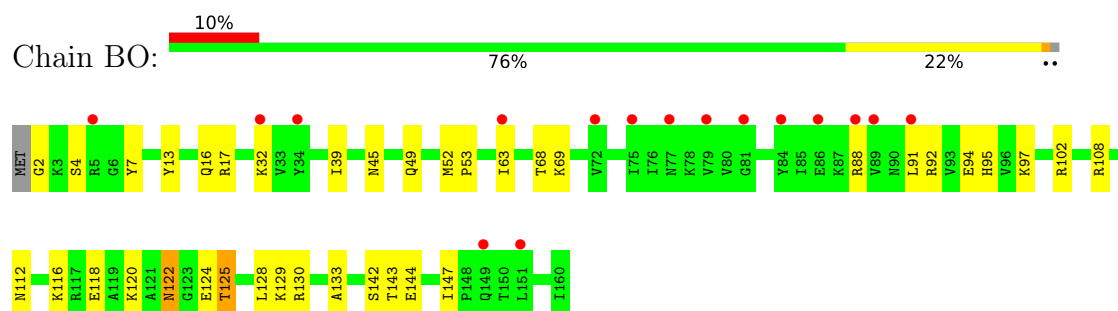
- Molecule 21: 60S ribosomal protein L20



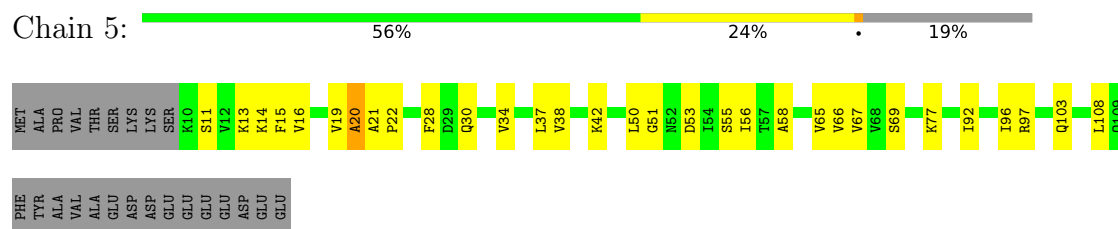
- Molecule 22: 60S ribosomal protein L21-A



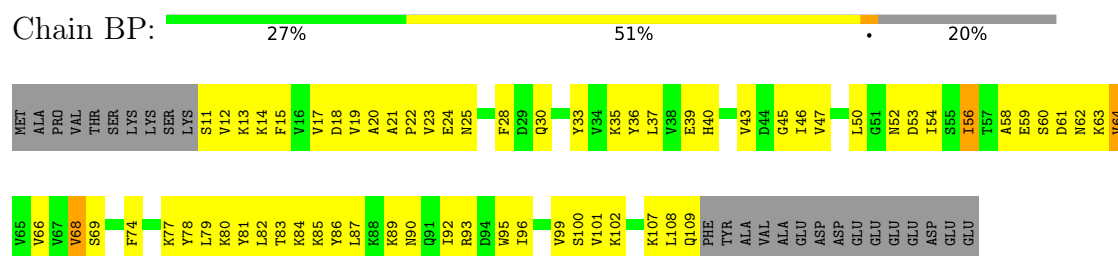
- Molecule 22: 60S ribosomal protein L21-A



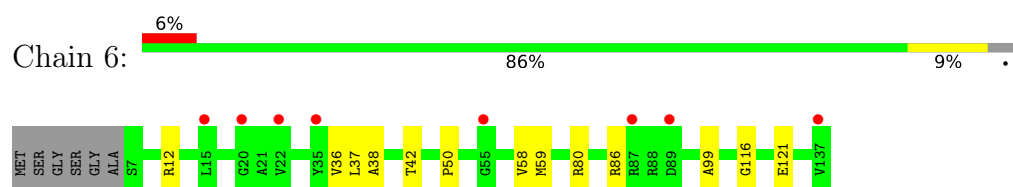
- Molecule 23: 60S ribosomal protein L22-B



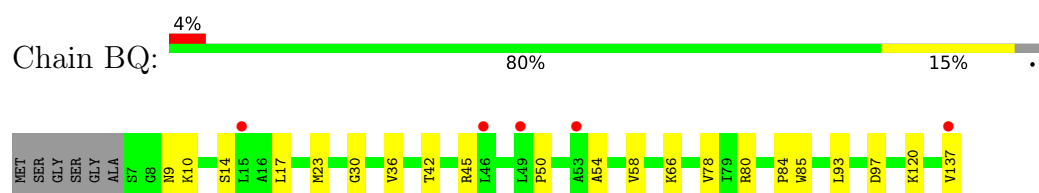
- Molecule 23: 60S ribosomal protein L22-B



- Molecule 24: 60S ribosomal protein L23-A



- Molecule 24: 60S ribosomal protein L23-A



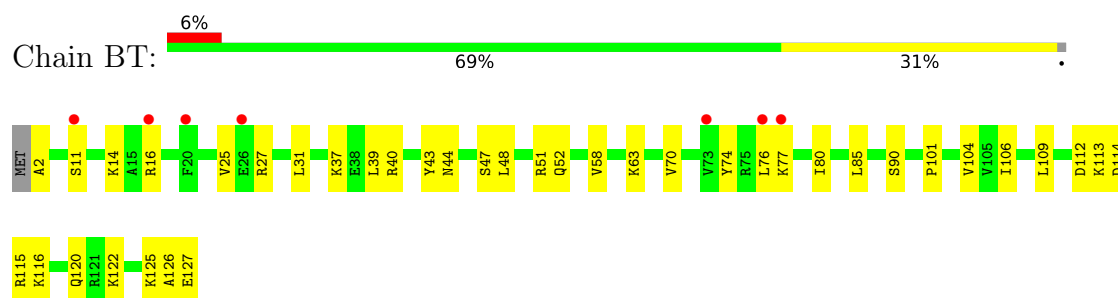
- Molecule 25: 60S ribosomal protein L24-A



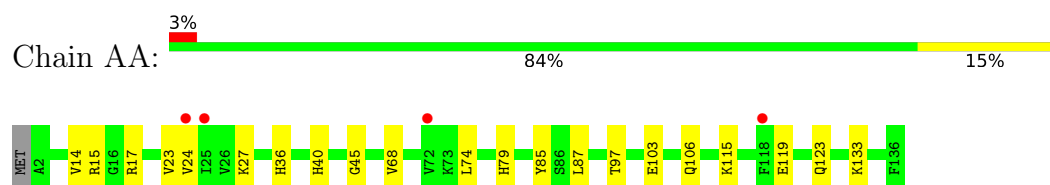




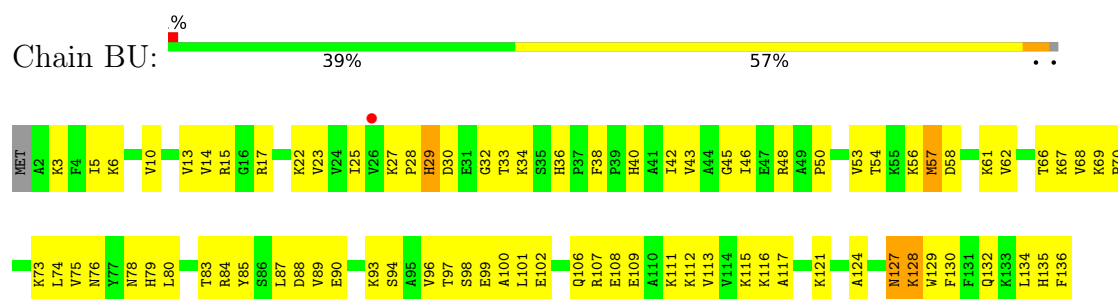
- Molecule 27: Ribosomal protein L24



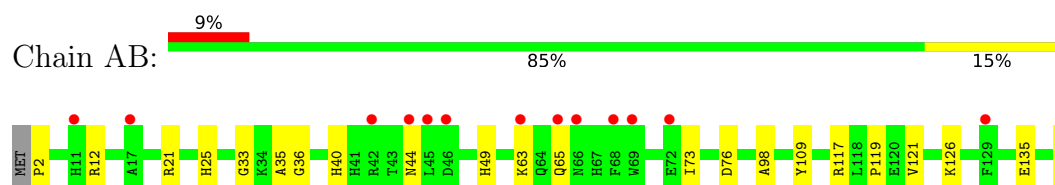
- Molecule 28: 60S ribosomal protein L27



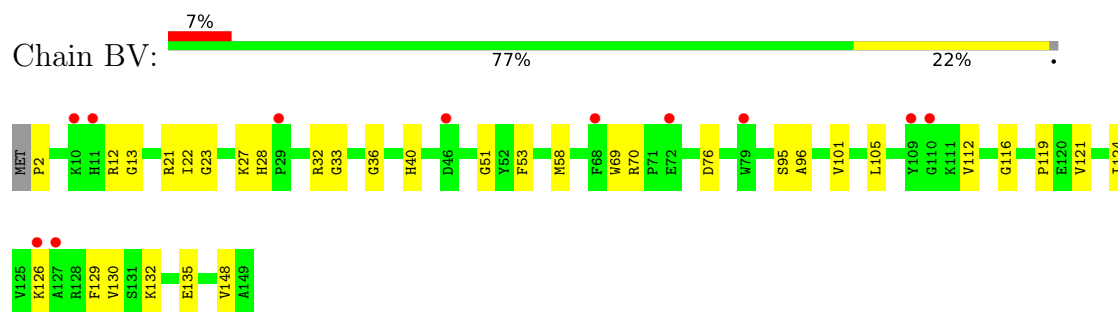
- Molecule 28: 60S ribosomal protein L27



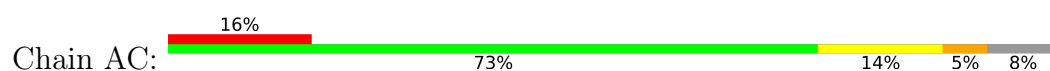
- Molecule 29: 60S ribosomal protein L28

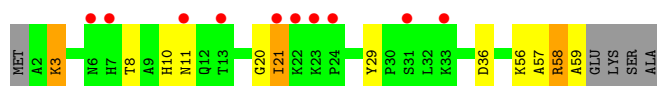


- Molecule 29: 60S ribosomal protein L28

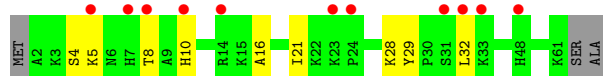
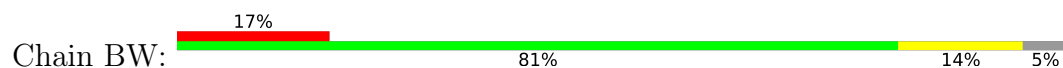


- Molecule 30: 60S ribosomal protein L29

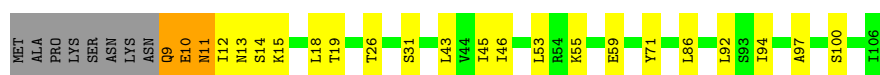




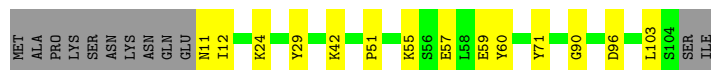
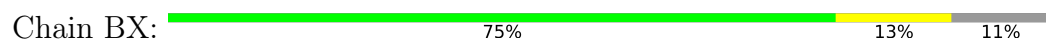
- Molecule 30: 60S ribosomal protein L29



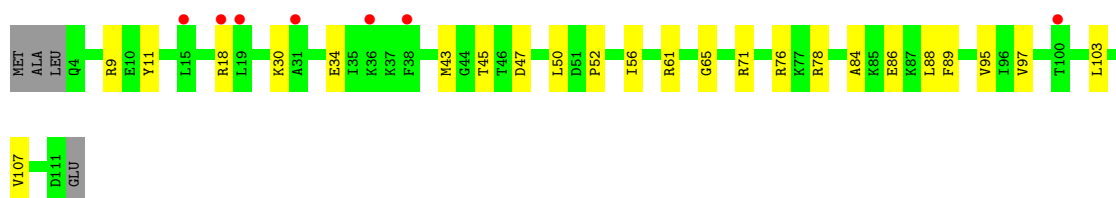
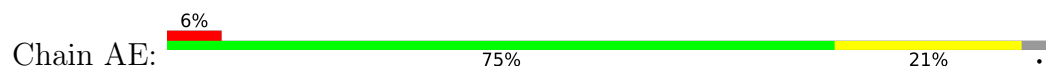
- Molecule 31: 60S ribosomal protein L30



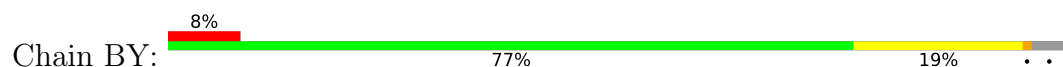
- Molecule 31: 60S ribosomal protein L30



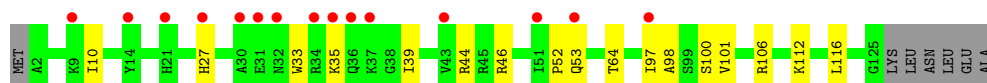
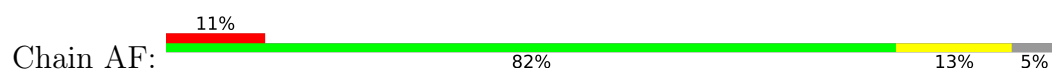
- Molecule 32: 60S ribosomal protein L31-B



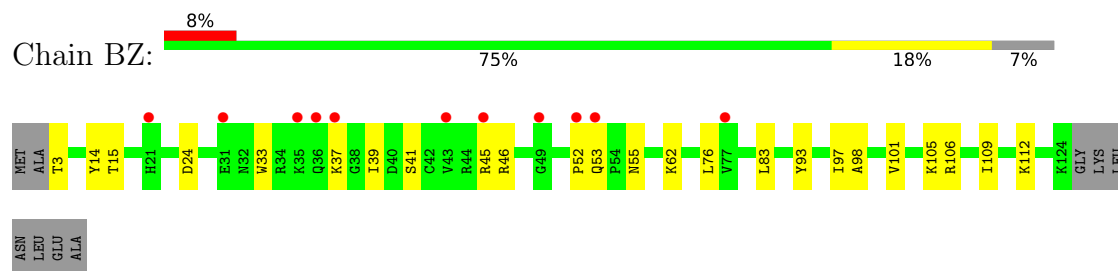
- Molecule 32: 60S ribosomal protein L31-B



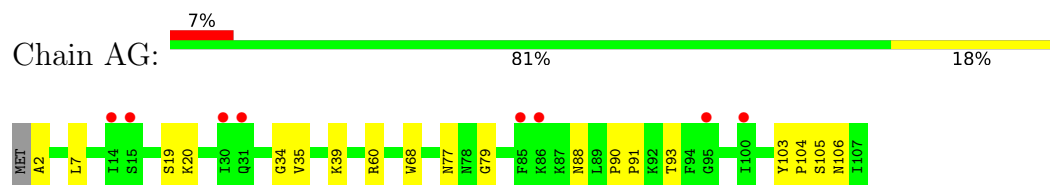
- Molecule 33: 60S ribosomal protein L32



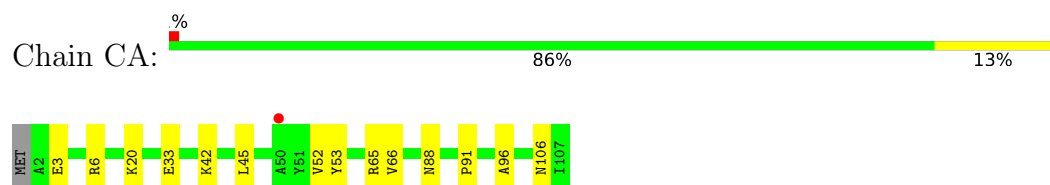
- Molecule 33: 60S ribosomal protein L32



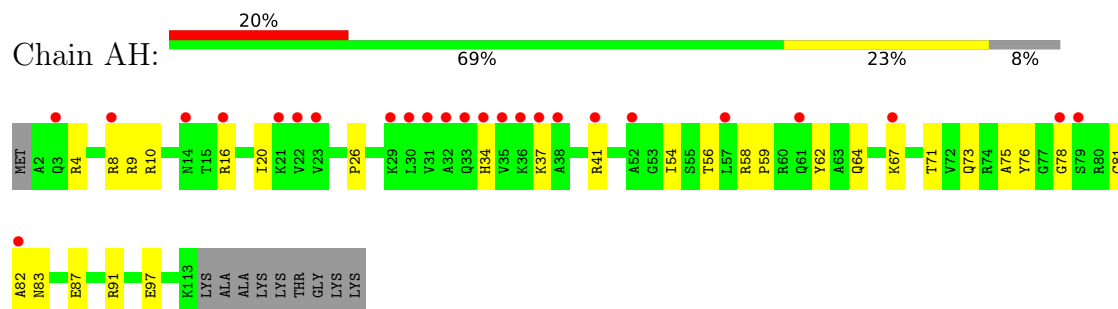
- Molecule 34: 60S ribosomal protein L33-A



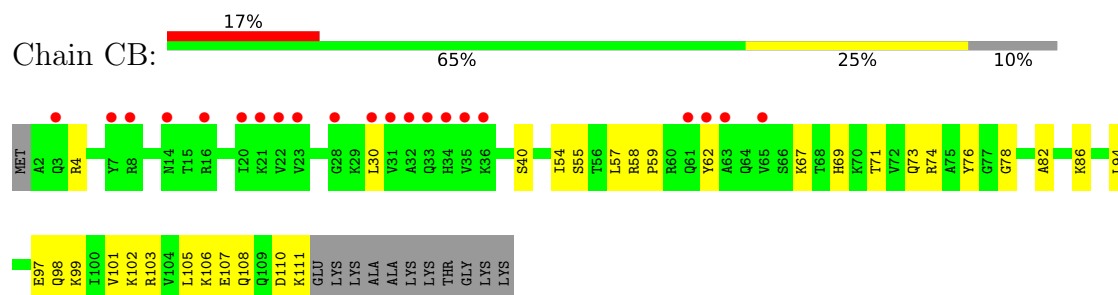
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-B



- Molecule 35: 60S ribosomal protein L34-B

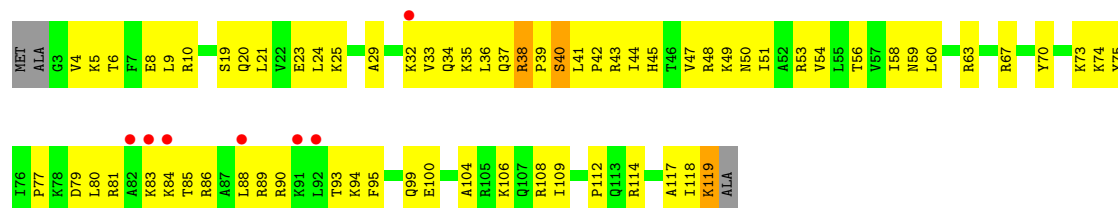
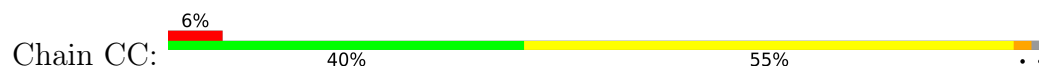


- Molecule 36: Ribosomal protein L29

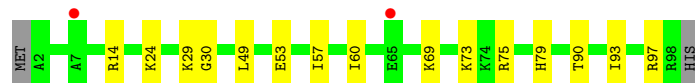
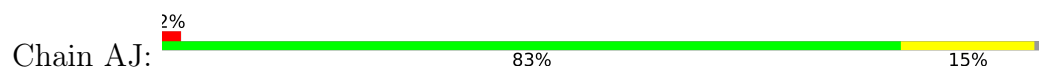




- Molecule 36: Ribosomal protein L29



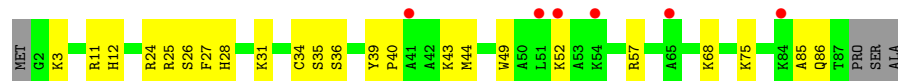
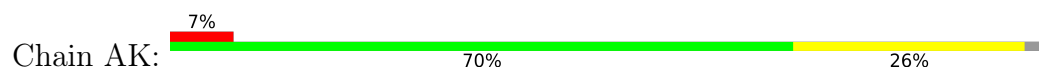
- Molecule 37: 60S ribosomal protein L36



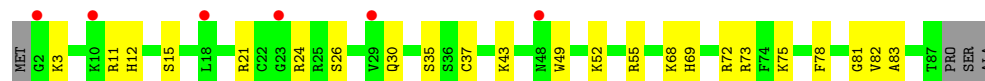
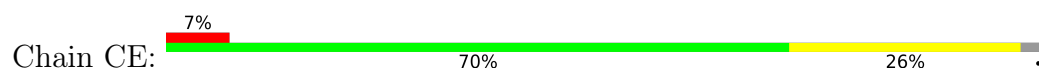
- Molecule 37: 60S ribosomal protein L36



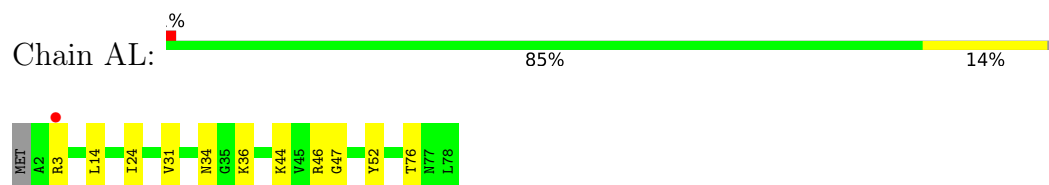
- Molecule 38: 60S ribosomal protein L37-B



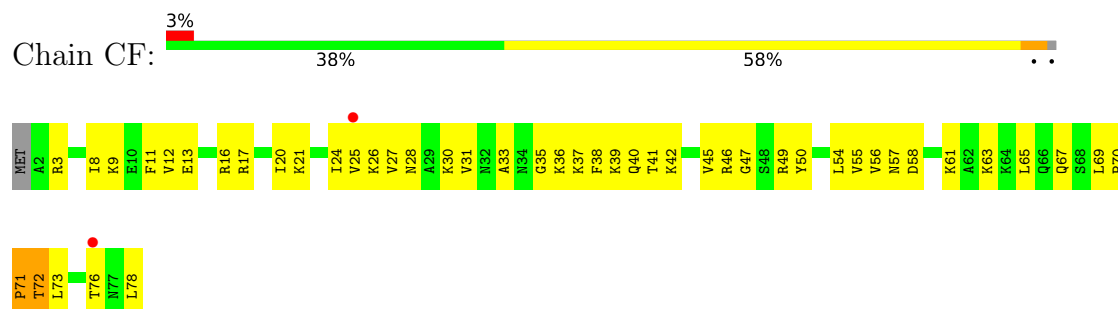
- Molecule 38: 60S ribosomal protein L37-B



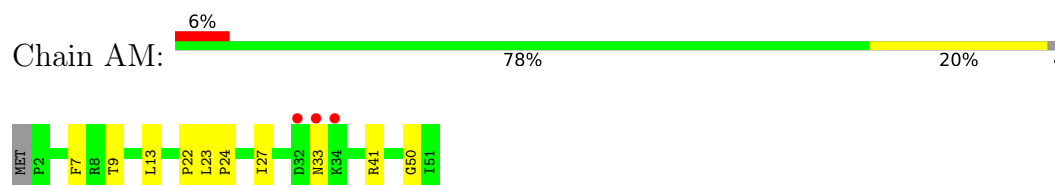
- Molecule 39: 60S ribosomal protein L38



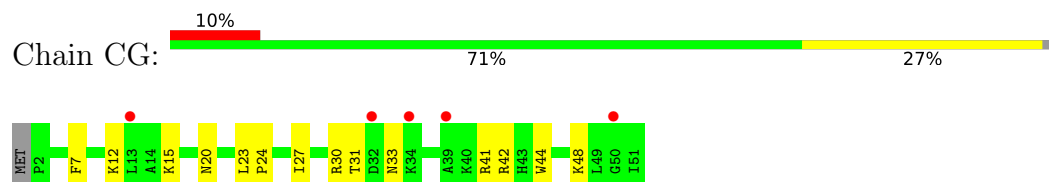
- Molecule 39: 60S ribosomal protein L38



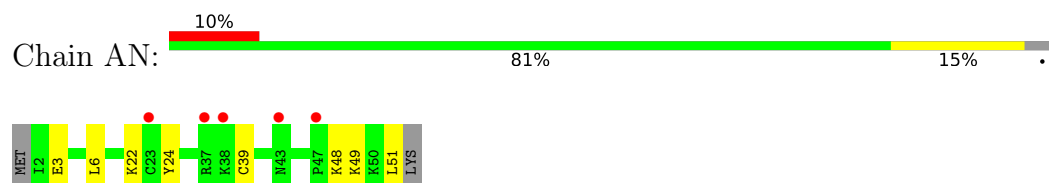
- Molecule 40: 60S ribosomal protein L39



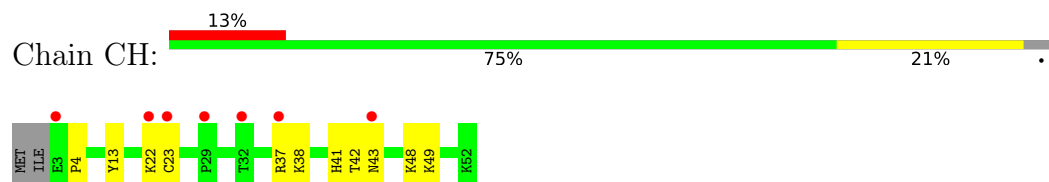
- Molecule 40: 60S ribosomal protein L39



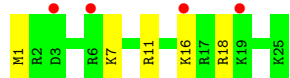
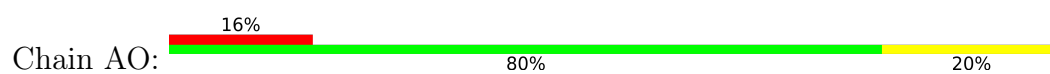
- Molecule 41: 60S ribosomal protein L40-B



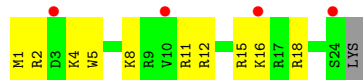
- Molecule 41: 60S ribosomal protein L40-B



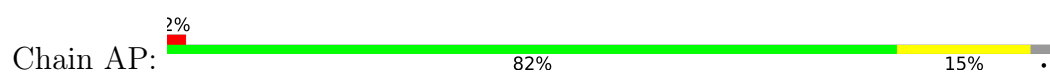
- Molecule 42: 60S ribosomal protein L41



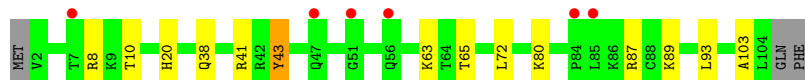
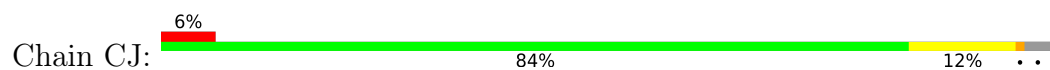
- Molecule 42: 60S ribosomal protein L41



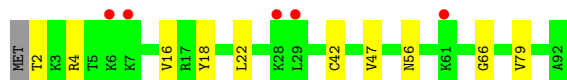
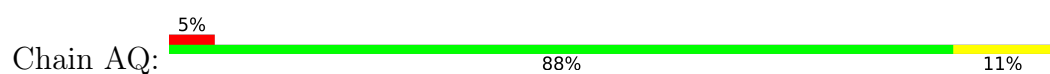
- Molecule 43: 60S ribosomal protein L42-B



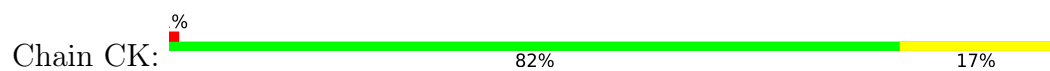
- Molecule 43: 60S ribosomal protein L42-B



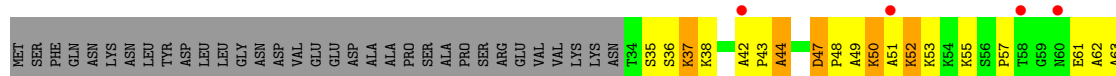
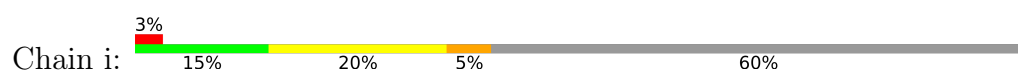
- Molecule 44: 60S ribosomal protein L43-A

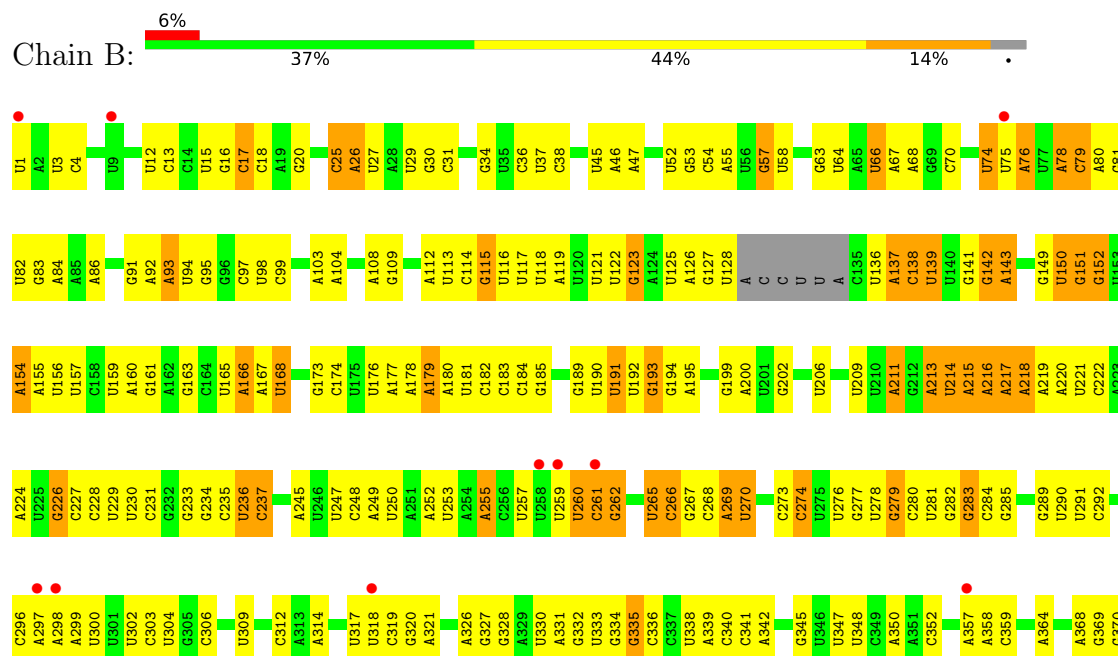


- Molecule 44: 60S ribosomal protein L43-A



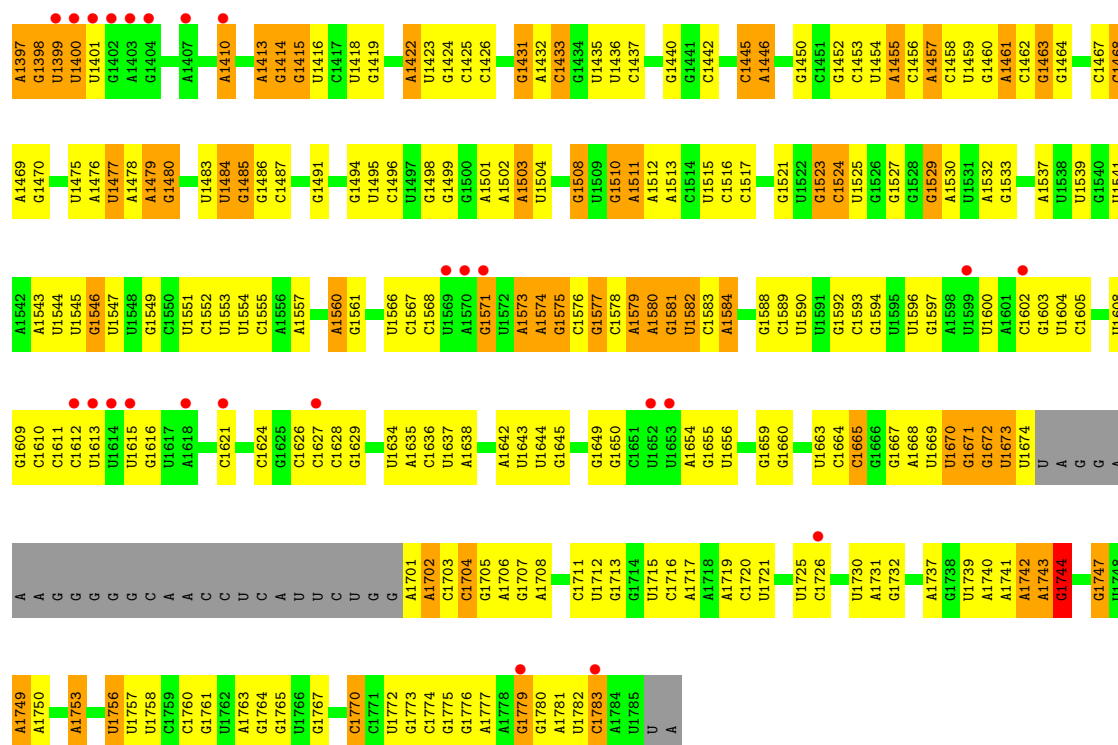
- Molecule 45: 60S ribosomal protein CAALFM\_C304810CA

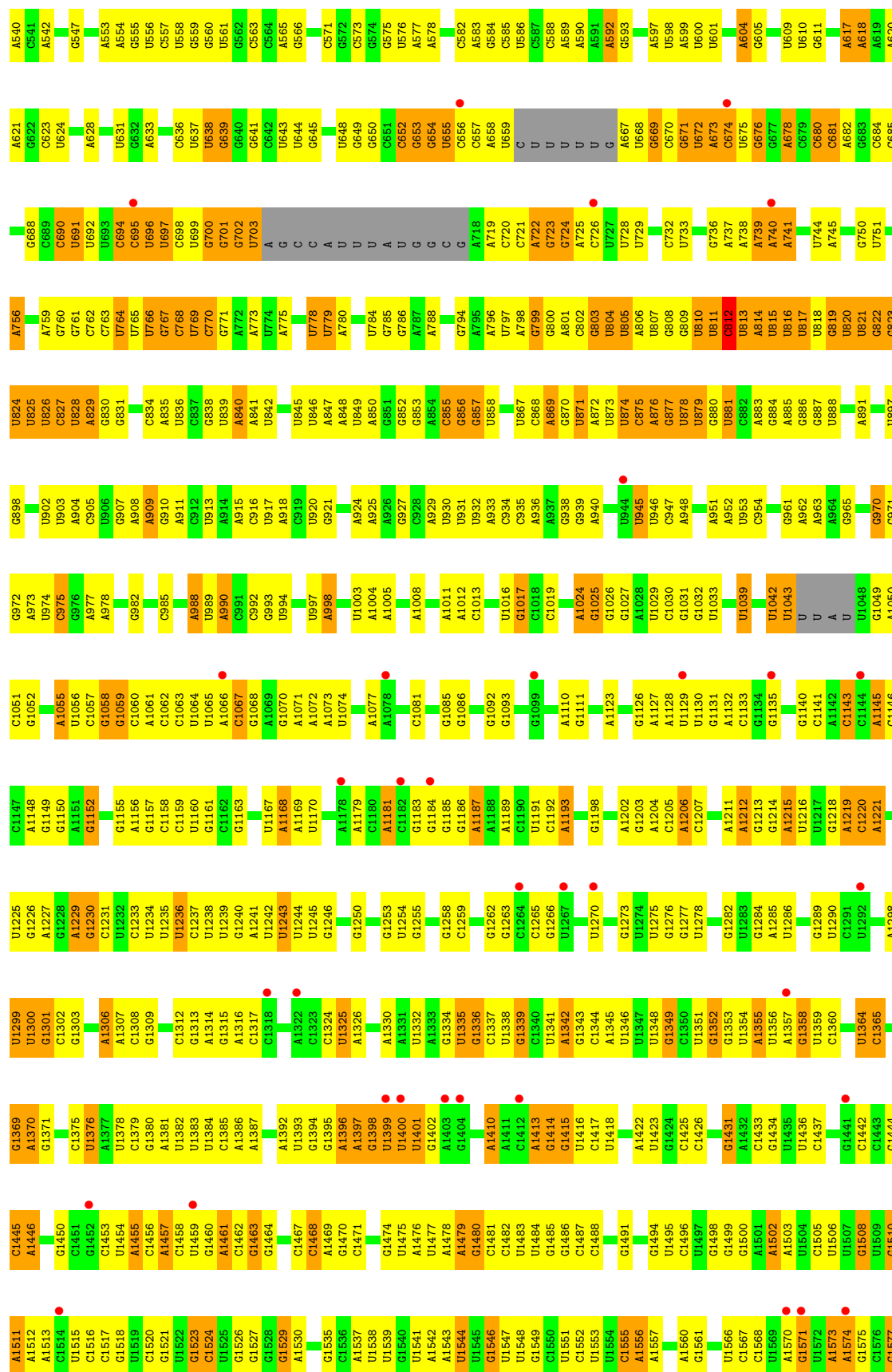


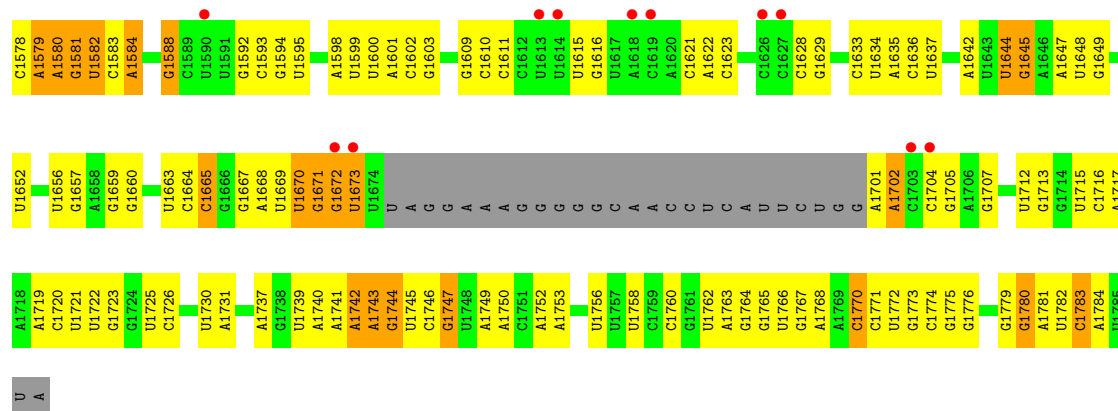




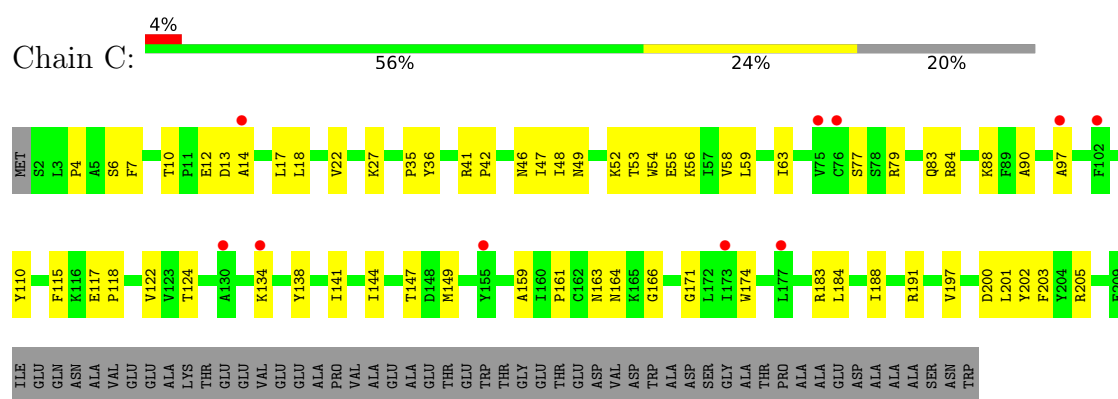




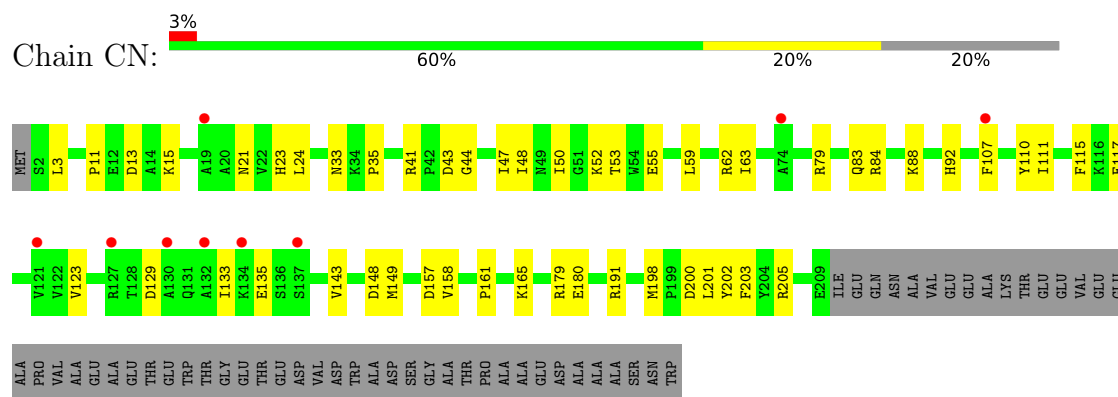




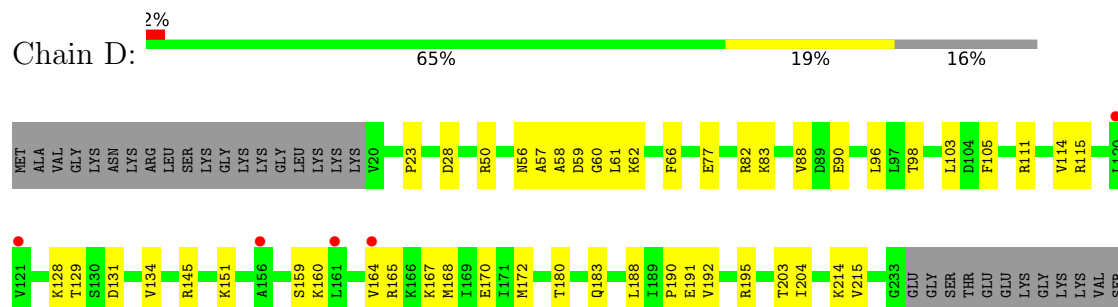
• Molecule 47: 40S ribosomal protein S0

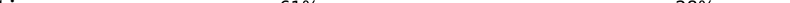


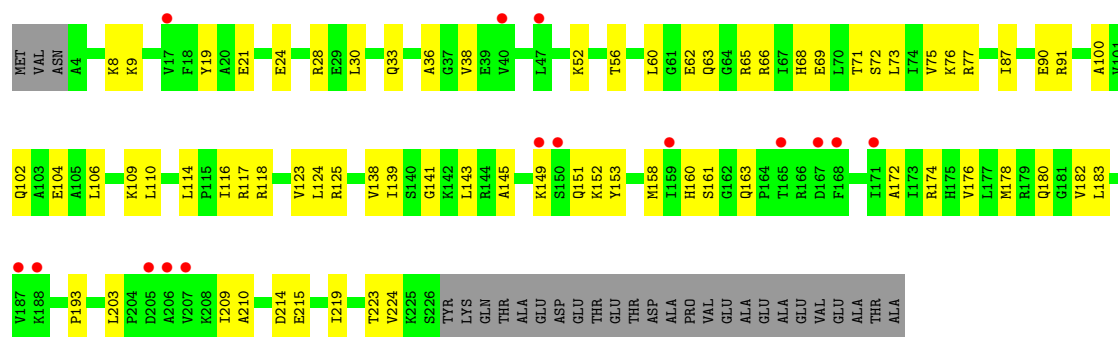
• Molecule 47: 40S ribosomal protein S0



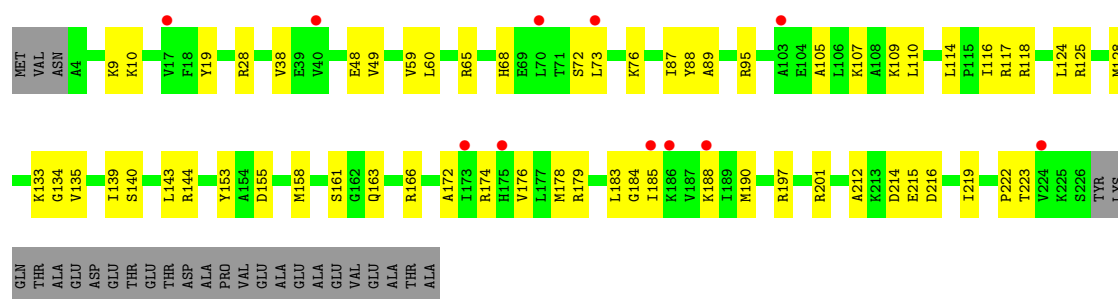
• Molecule 48: 40S ribosomal protein S1



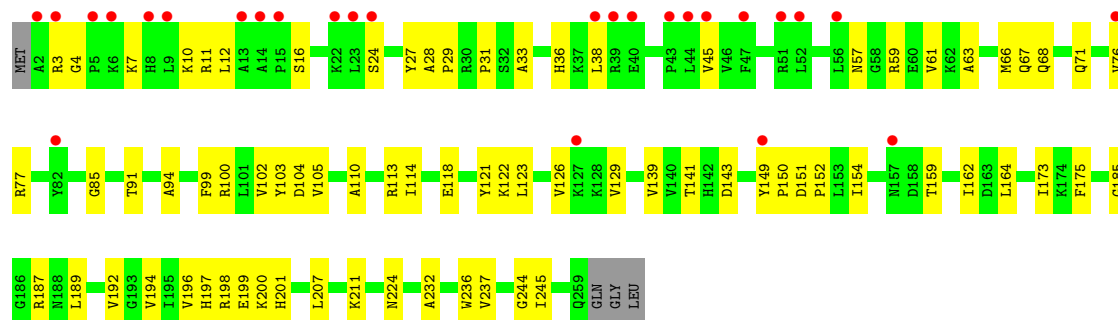
Chain F: 



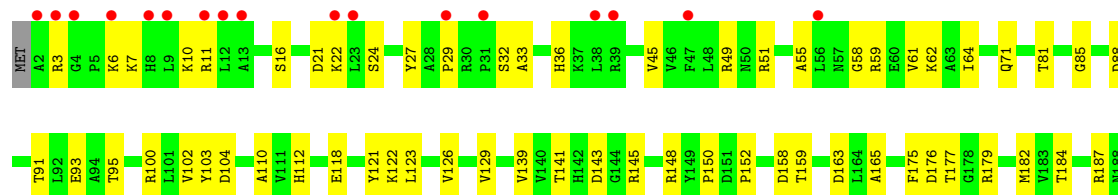
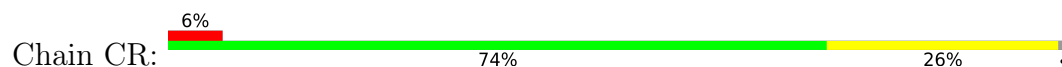
• Molecule 50: Ribosomal protein S3



• Molecule 51: 40S ribosomal protein S4

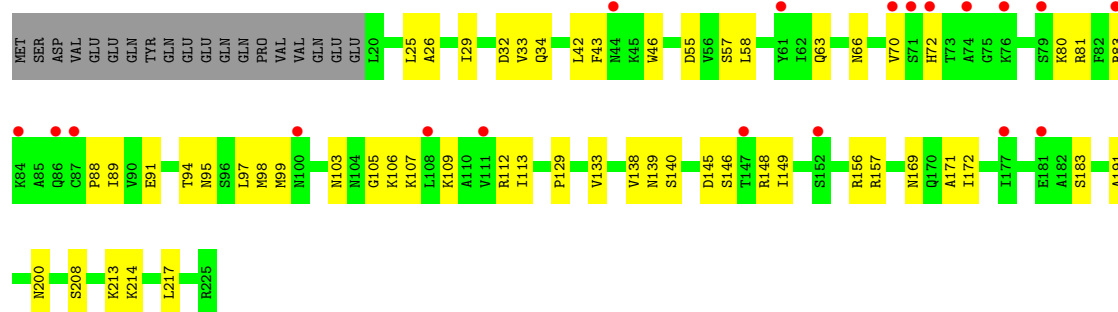


• Molecule 51: 40S ribosomal protein S4

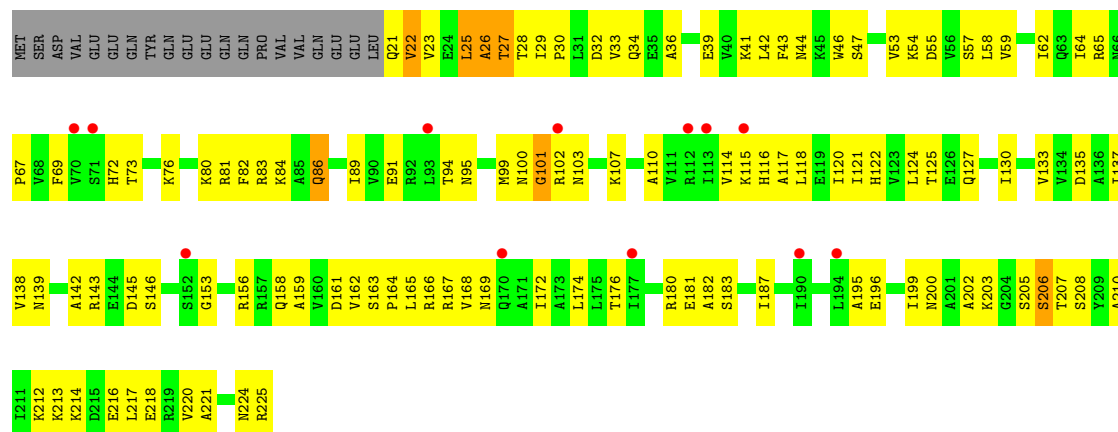




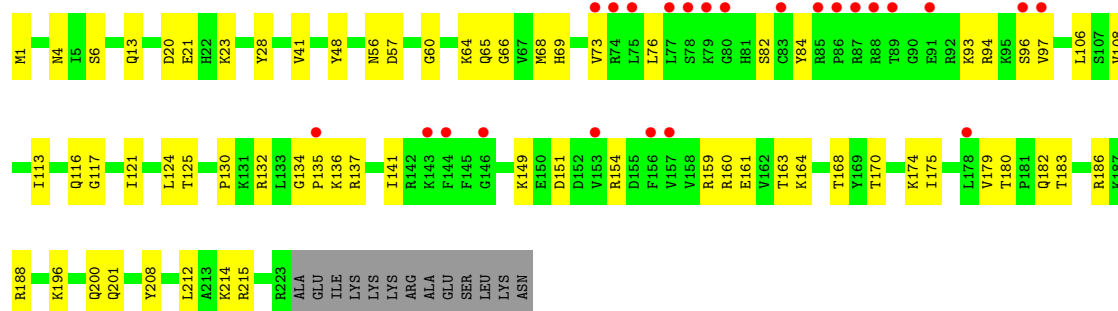
• Molecule 52: Ribosomal protein S7



• Molecule 52: Ribosomal protein S7

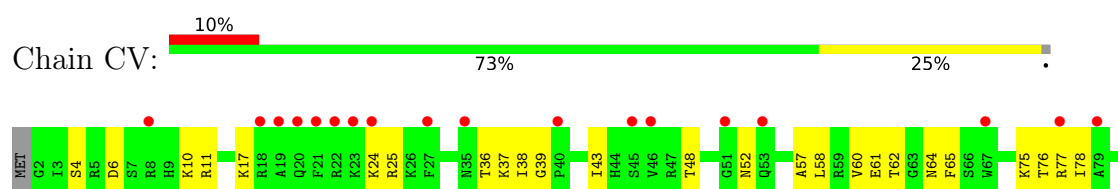


• Molecule 53: 40S ribosomal protein S6

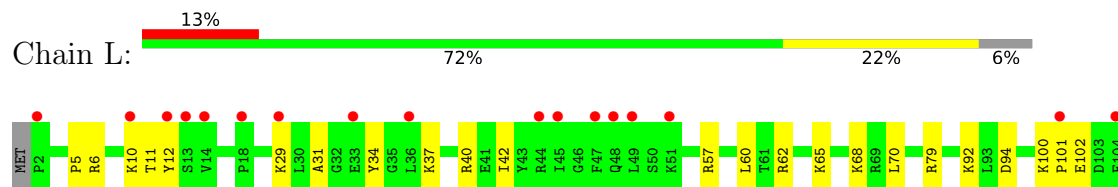


• Molecule 53: 40S ribosomal protein S6

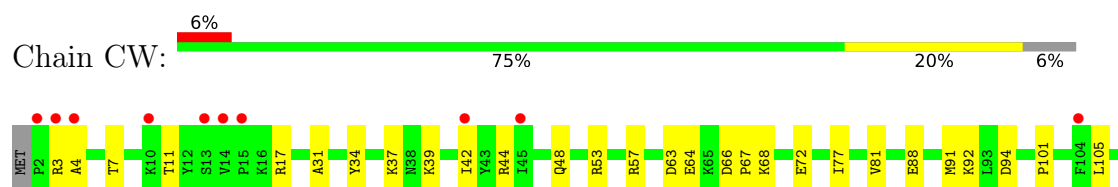




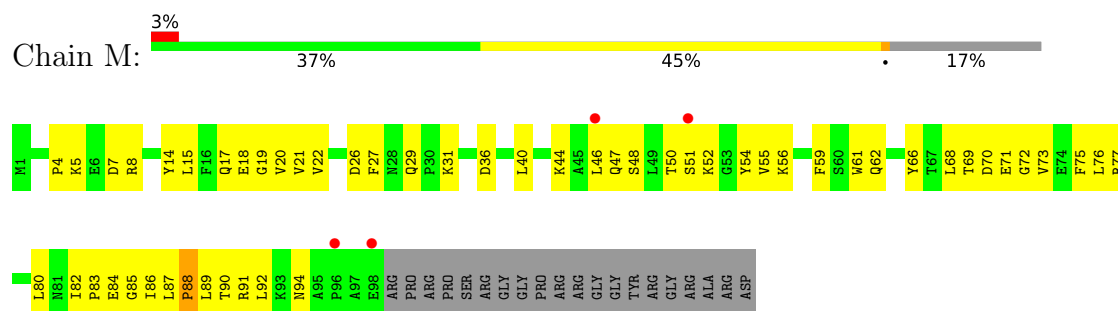
- Molecule 56: Ribosomal protein S4



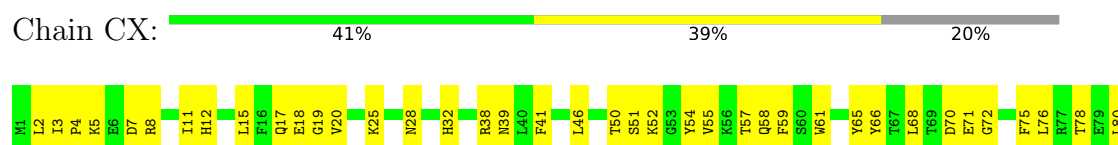
- Molecule 56: Ribosomal protein S4



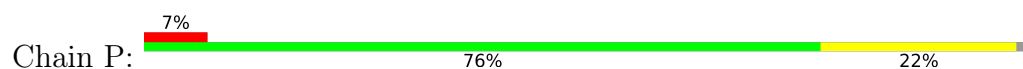
- Molecule 57: 40S ribosomal protein S10-A

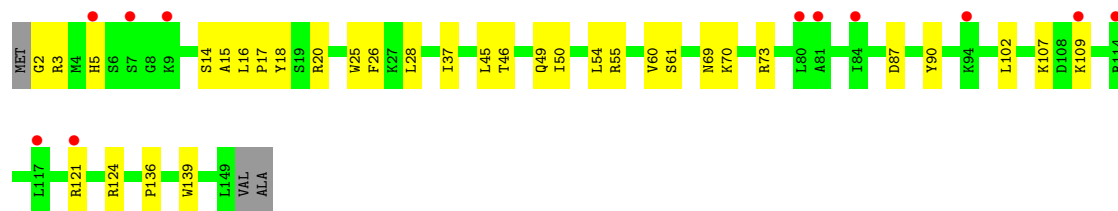


- Molecule 57: 40S ribosomal protein S10-A

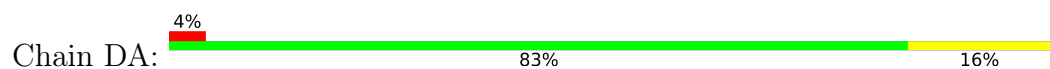




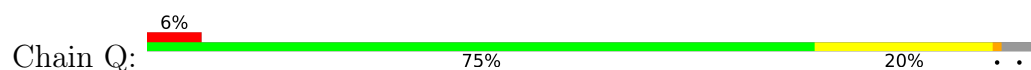




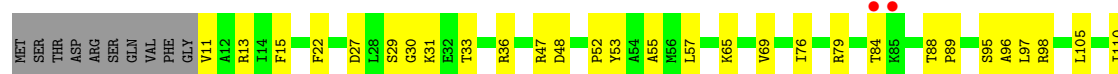
- Molecule 60: 40S ribosomal protein S13



- Molecule 61: 40S ribosomal protein S14-A



- Molecule 61: 40S ribosomal protein S14-A

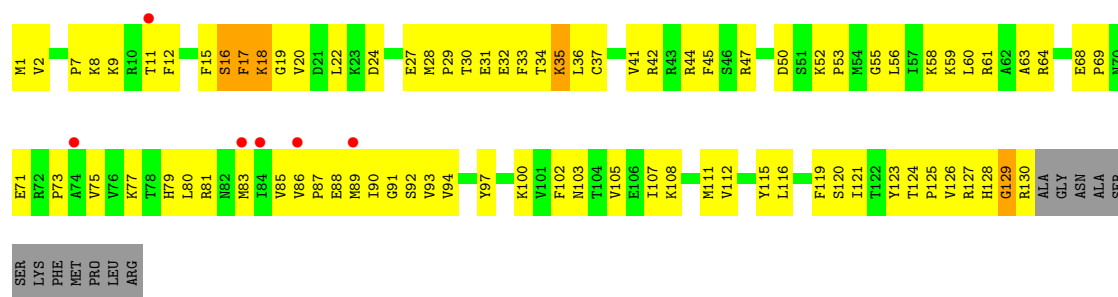


- Molecule 62: 40S ribosomal protein S15

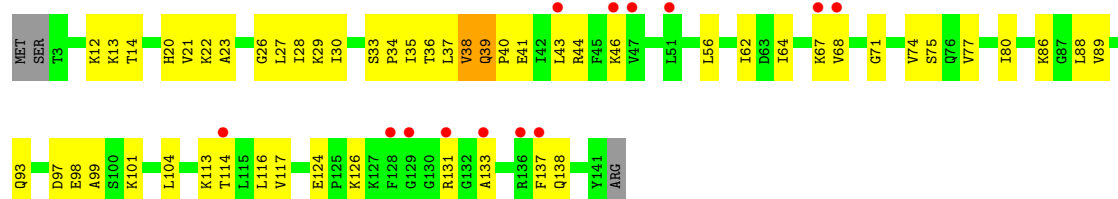


- Molecule 62: 40S ribosomal protein S15

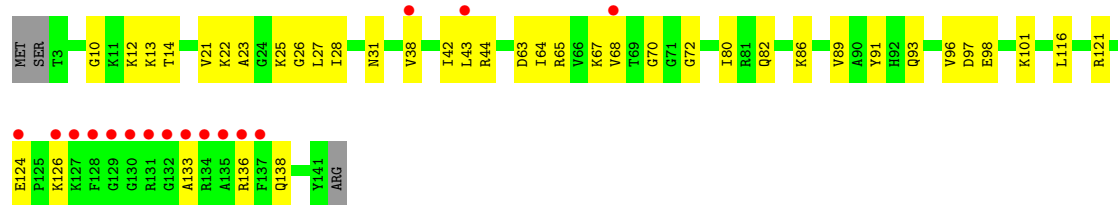
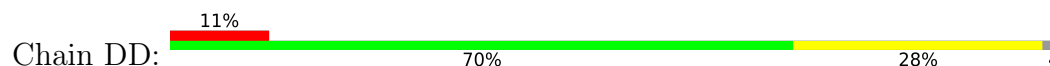




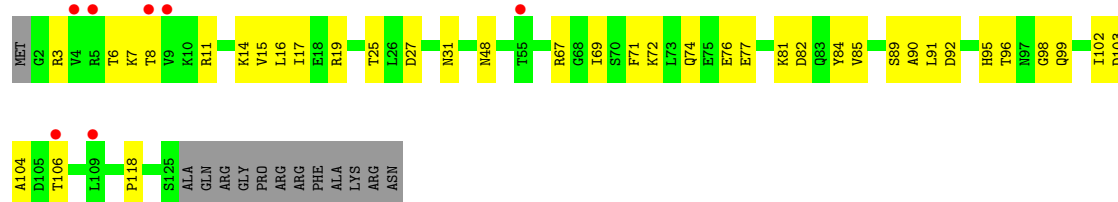
- Molecule 63: 40S ribosomal protein S16



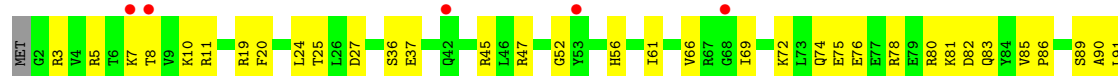
- Molecule 63: 40S ribosomal protein S16

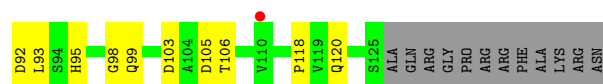


- Molecule 64: 40S ribosomal protein S17-B

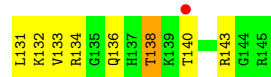
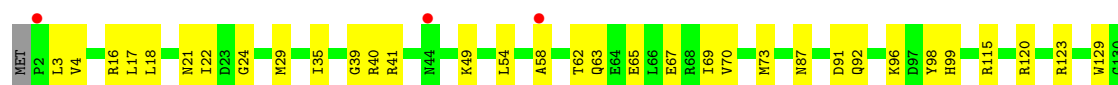


- Molecule 64: 40S ribosomal protein S17-B

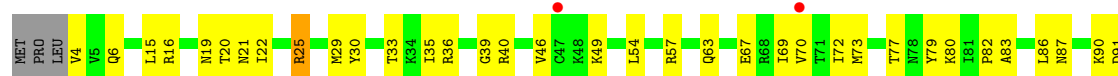




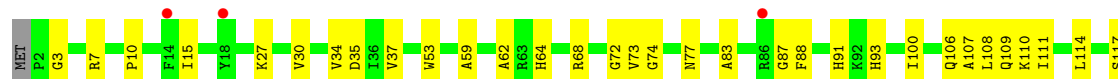
- Molecule 65: 40S ribosomal protein S18-B



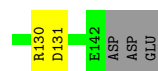
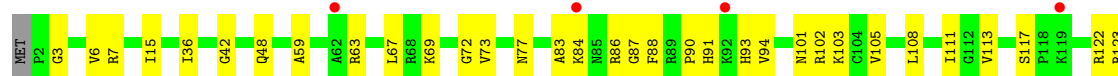
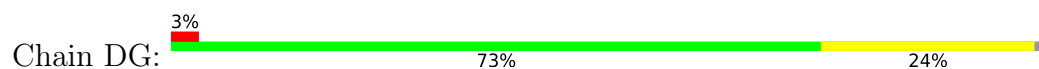
- Molecule 65: 40S ribosomal protein S18-B



- Molecule 66: 40S ribosomal protein S19-A



- Molecule 66: 40S ribosomal protein S19-A



- Molecule 67: Ribosomal protein S10

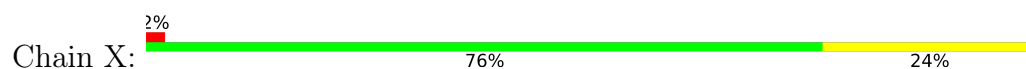




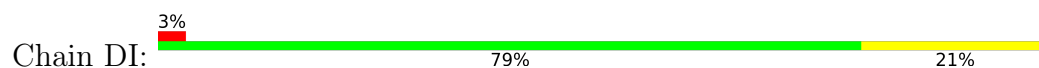
• Molecule 67: Ribosomal protein S10



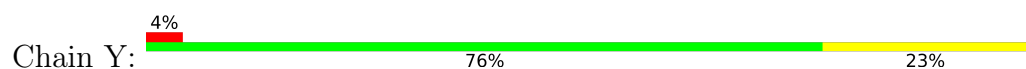
• Molecule 68: 40S ribosomal protein S21



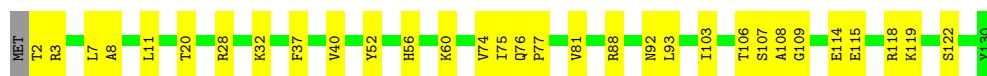
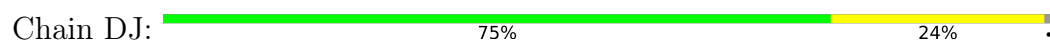
• Molecule 68: 40S ribosomal protein S21



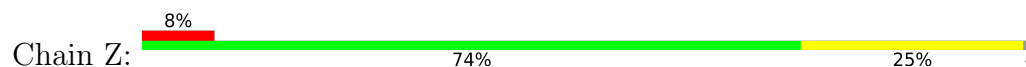
• Molecule 69: 40S ribosomal protein S22-A

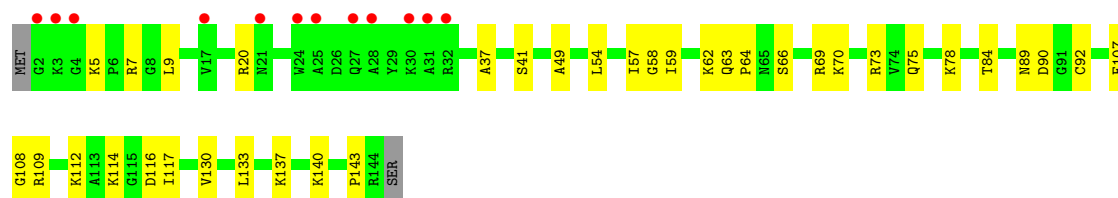


• Molecule 69: 40S ribosomal protein S22-A

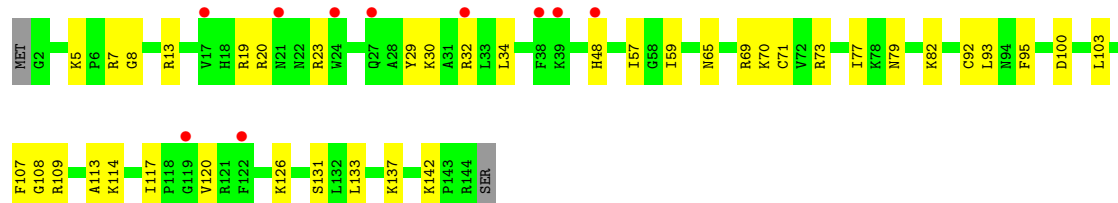
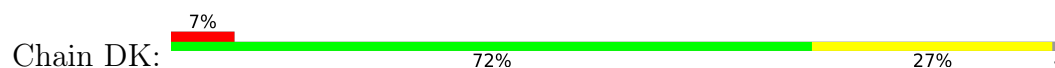


• Molecule 70: Ribosomal protein S23 (S12)

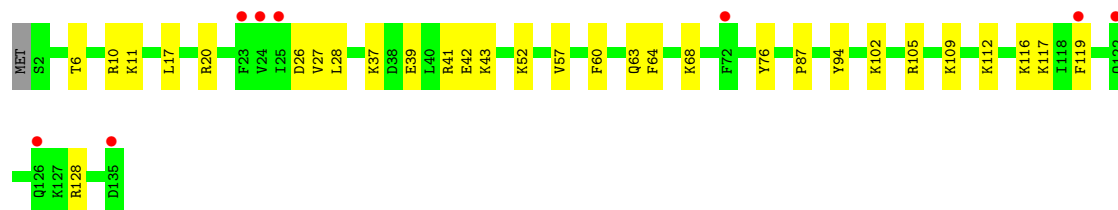
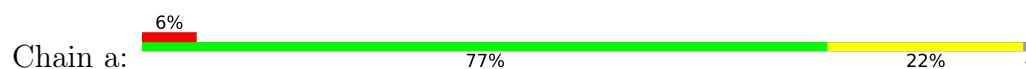




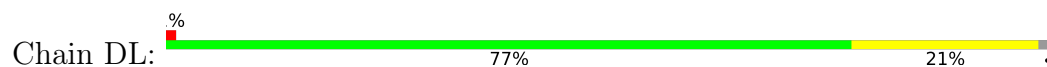
- Molecule 70: Ribosomal protein S23 (S12)



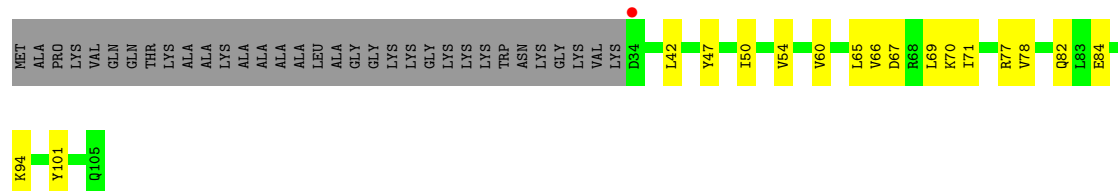
- Molecule 71: 40S ribosomal protein S24



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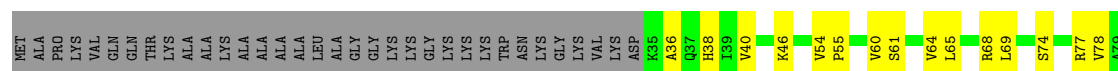


- Molecule 72: 40S ribosomal protein S25



- Molecule 72: 40S ribosomal protein S25

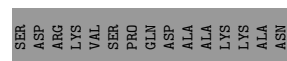




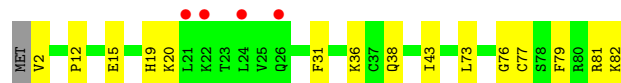
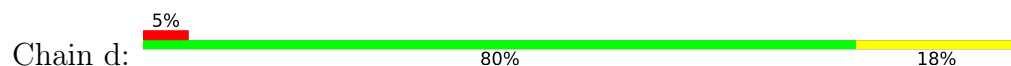
- Molecule 73: 40S ribosomal protein S26



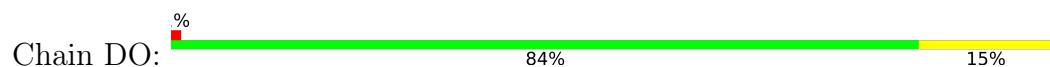
- Molecule 73: 40S ribosomal protein S26



- Molecule 74: 40S ribosomal protein S27



- Molecule 74: 40S ribosomal protein S27



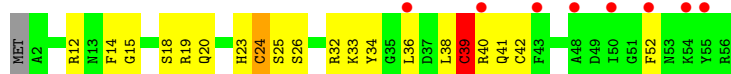
- Molecule 75: 40S ribosomal protein S28-B



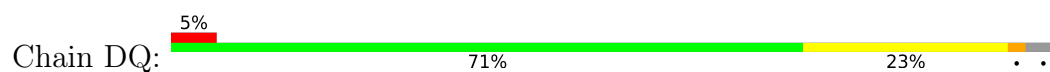
- Molecule 75: 40S ribosomal protein S28-B



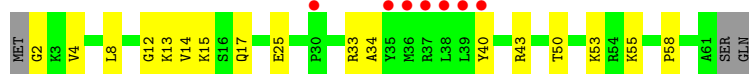
- Molecule 76: 40S ribosomal protein S29A



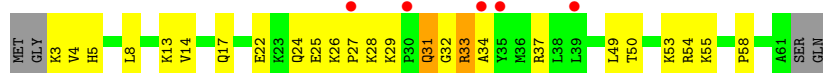
- Molecule 76: 40S ribosomal protein S29A



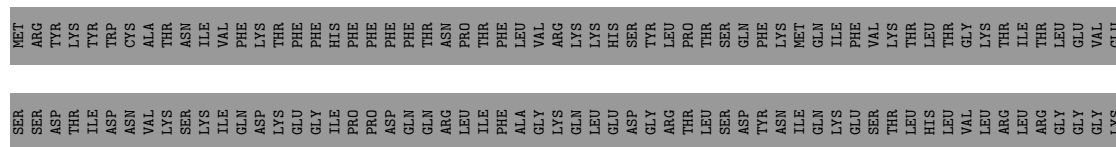
- Molecule 77: 40S ribosomal protein S30



- Molecule 77: 40S ribosomal protein S30

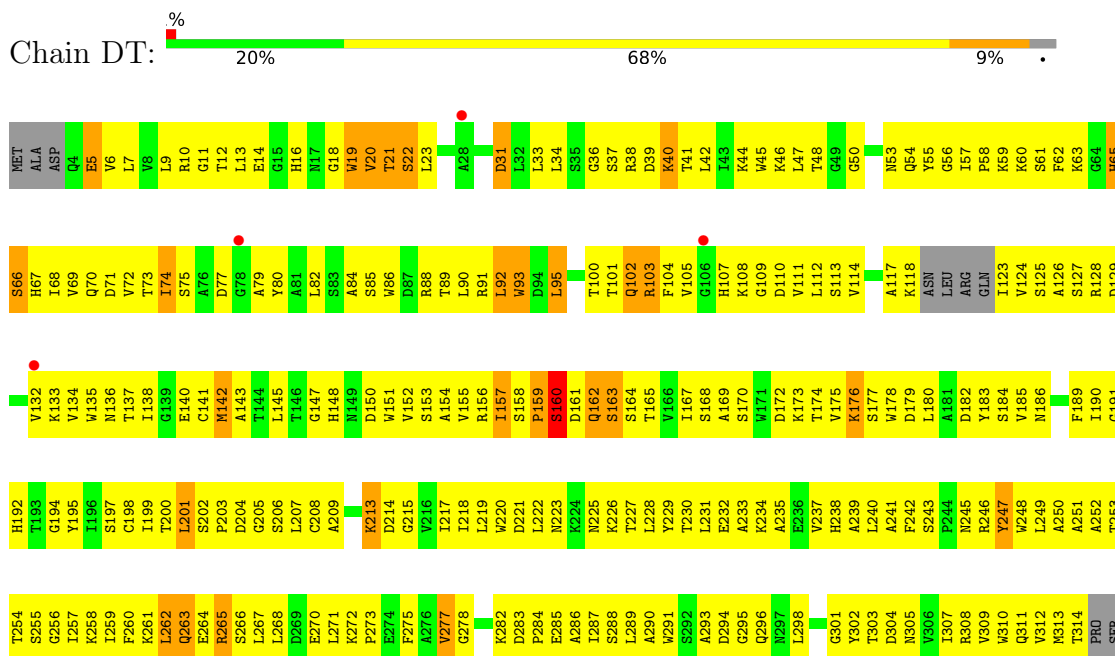
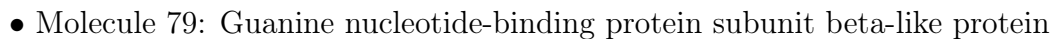
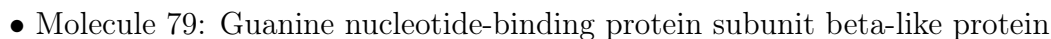


- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein



- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein







## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 300.29Å 294.06Å 442.55Å<br>90.00° 99.77° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 266.82 – 3.50<br>266.82 – 3.50                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.9 (266.82-3.50)<br>86.6 (266.82-3.50)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.52                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.69 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.19rc4_4035                                         | Depositor        |
| R, $R_{free}$                                                           | 0.249 , 0.293<br>0.249 , 0.291                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (0.16%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.138                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 91.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 400037                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 132.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GET, ZN, 3K5, MG

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   | 1     | 0.20         | 0/76993     | 0.48        | 17/120031 (0.0%) |
| 1   | AS    | 0.20         | 0/74190     | 0.48        | 11/115649 (0.0%) |
| 2   | 3     | 0.16         | 0/2884      | 0.36        | 0/4492           |
| 2   | AT    | 0.18         | 0/2884      | 0.37        | 0/4492           |
| 3   | 4     | 0.16         | 0/3702      | 0.41        | 0/5764           |
| 3   | AU    | 0.21         | 0/3746      | 0.49        | 4/5832 (0.1%)    |
| 4   | AW    | 0.16         | 0/1922      | 0.44        | 0/2581           |
| 4   | j     | 0.17         | 0/1922      | 0.46        | 0/2581           |
| 5   | AX    | 0.21         | 0/3145      | 0.52        | 2/4231 (0.0%)    |
| 5   | k     | 0.20         | 0/3145      | 0.51        | 0/4231           |
| 6   | AY    | 0.16         | 0/2782      | 0.47        | 0/3754           |
| 6   | l     | 0.18         | 0/2782      | 0.51        | 0/3754           |
| 7   | AZ    | 0.17         | 0/2447      | 0.45        | 0/3294           |
| 7   | m     | 0.17         | 0/2462      | 0.48        | 0/3315           |
| 8   | BA    | 0.17         | 0/1231      | 0.50        | 0/1662           |
| 8   | n     | 0.18         | 0/1263      | 0.50        | 0/1703           |
| 9   | BB    | 0.16         | 0/1849      | 0.48        | 0/2485           |
| 9   | o     | 0.19         | 0/1876      | 0.49        | 0/2519           |
| 10  | BC    | 0.48         | 0/1835      | 1.00        | 1/2472 (0.0%)    |
| 10  | p     | 0.25         | 0/1855      | 0.62        | 3/2500 (0.1%)    |
| 11  | BD    | 0.18         | 0/1537      | 0.46        | 0/2067           |
| 11  | q     | 0.19         | 0/1537      | 0.49        | 0/2067           |
| 12  | r     | 0.19         | 0/1716      | 0.47        | 0/2304           |
| 13  | BF    | 0.18         | 0/1390      | 0.50        | 0/1861           |
| 13  | s     | 0.18         | 0/1390      | 0.51        | 0/1861           |
| 14  | BG    | 0.47         | 0/1637      | 0.99        | 6/2195 (0.3%)    |
| 14  | t     | 0.24         | 0/1637      | 0.63        | 3/2195 (0.1%)    |
| 15  | BH    | 0.18         | 0/1044      | 0.47        | 0/1407           |
| 15  | u     | 0.22         | 0/1030      | 0.49        | 0/1389           |
| 16  | BI    | 0.17         | 0/1753      | 0.46        | 0/2347           |
| 16  | v     | 0.17         | 0/1753      | 0.47        | 0/2347           |
| 17  | BJ    | 0.20         | 0/1620      | 0.46        | 0/2167           |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 17  | w     | 0.20         | 0/1620        | 0.51        | 0/2167        |
| 18  | BK    | 0.16         | 0/1419        | 0.45        | 0/1906        |
| 18  | x     | 0.23         | 0/1375        | 0.56        | 0/1848        |
| 19  | BL    | 0.16         | 0/1482        | 0.46        | 0/1985        |
| 19  | y     | 0.24         | 1/1482 (0.1%) | 0.46        | 0/1985        |
| 20  | BM    | 0.25         | 0/1475        | 0.63        | 0/1961        |
| 20  | z     | 0.30         | 0/1475        | 0.66        | 2/1961 (0.1%) |
| 21  | 0     | 0.18         | 0/1457        | 0.47        | 0/1962        |
| 21  | BN    | 0.17         | 0/1457        | 0.42        | 0/1962        |
| 22  | 2     | 0.16         | 0/1285        | 0.45        | 0/1723        |
| 22  | BO    | 0.33         | 0/1285        | 0.72        | 2/1723 (0.1%) |
| 23  | 5     | 0.24         | 0/816         | 0.62        | 0/1099        |
| 23  | BP    | 0.48         | 0/807         | 1.10        | 1/1088 (0.1%) |
| 24  | 6     | 0.17         | 0/993         | 0.48        | 0/1339        |
| 24  | BQ    | 0.18         | 0/993         | 0.48        | 0/1339        |
| 25  | 7     | 0.29         | 0/958         | 0.53        | 0/1267        |
| 25  | BR    | 0.26         | 0/889         | 0.57        | 1/1175 (0.1%) |
| 26  | 8     | 0.19         | 0/981         | 0.49        | 0/1326        |
| 26  | BS    | 0.55         | 0/976         | 1.02        | 4/1319 (0.3%) |
| 27  | 9     | 0.26         | 0/999         | 0.57        | 0/1334        |
| 27  | BT    | 0.17         | 0/999         | 0.47        | 0/1334        |
| 28  | AA    | 0.15         | 0/1112        | 0.41        | 0/1488        |
| 28  | BU    | 0.52         | 1/1112 (0.1%) | 1.05        | 5/1488 (0.3%) |
| 29  | AB    | 0.15         | 0/1199        | 0.46        | 0/1607        |
| 29  | BV    | 0.17         | 0/1199        | 0.46        | 0/1607        |
| 30  | AC    | 0.21         | 0/474         | 0.71        | 0/630         |
| 30  | BW    | 0.21         | 0/492         | 0.50        | 0/653         |
| 31  | AD    | 0.23         | 0/756         | 0.46        | 0/1018        |
| 31  | BX    | 0.15         | 0/724         | 0.45        | 0/975         |
| 32  | AE    | 0.17         | 0/894         | 0.47        | 0/1201        |
| 32  | BY    | 0.15         | 0/894         | 0.48        | 0/1201        |
| 33  | AF    | 0.16         | 0/1021        | 0.48        | 0/1368        |
| 33  | BZ    | 0.17         | 0/1012        | 0.51        | 0/1356        |
| 34  | AG    | 0.17         | 0/866         | 0.47        | 0/1165        |
| 34  | CA    | 0.20         | 0/866         | 0.43        | 0/1165        |
| 35  | AH    | 0.17         | 0/896         | 0.47        | 0/1195        |
| 35  | CB    | 0.23         | 0/878         | 0.58        | 0/1172        |
| 36  | AI    | 0.16         | 0/974         | 0.47        | 0/1297        |
| 36  | CC    | 0.50         | 0/985         | 0.97        | 1/1312 (0.1%) |
| 37  | AJ    | 0.15         | 0/763         | 0.43        | 0/1012        |
| 37  | CD    | 0.49         | 0/741         | 1.08        | 1/984 (0.1%)  |
| 38  | AK    | 0.18         | 0/690         | 0.52        | 0/916         |
| 38  | CE    | 0.18         | 0/690         | 0.50        | 0/916         |

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 39  | AL    | 0.13         | 0/623         | 0.46        | 0/831           |
| 39  | CF    | 0.50         | 0/623         | 0.99        | 0/831           |
| 40  | AM    | 0.17         | 0/447         | 0.46        | 0/594           |
| 40  | CG    | 0.18         | 0/447         | 0.51        | 0/594           |
| 41  | AN    | 0.14         | 0/408         | 0.42        | 0/542           |
| 41  | CH    | 0.25         | 0/409         | 0.50        | 0/542           |
| 42  | AO    | 0.20         | 0/237         | 0.48        | 0/304           |
| 42  | CI    | 0.22         | 0/228         | 0.44        | 0/293           |
| 43  | AP    | 0.18         | 0/840         | 0.49        | 0/1110          |
| 43  | CJ    | 0.17         | 0/840         | 0.53        | 1/1110 (0.1%)   |
| 44  | AQ    | 0.18         | 0/705         | 0.48        | 0/940           |
| 44  | CK    | 0.16         | 0/705         | 0.45        | 0/940           |
| 45  | CL    | 0.48         | 0/929         | 1.13        | 5/1240 (0.4%)   |
| 45  | i     | 0.53         | 0/816         | 1.24        | 6/1091 (0.5%)   |
| 46  | B     | 0.20         | 0/40724       | 0.50        | 8/63452 (0.0%)  |
| 46  | CM    | 0.22         | 0/41205       | 0.52        | 14/64202 (0.0%) |
| 47  | C     | 0.16         | 0/1666        | 0.44        | 0/2273          |
| 47  | CN    | 0.16         | 0/1666        | 0.46        | 0/2273          |
| 48  | CO    | 0.63         | 0/1743        | 1.17        | 4/2344 (0.2%)   |
| 48  | D     | 0.18         | 0/1750        | 0.51        | 0/2354          |
| 49  | CP    | 0.15         | 0/1657        | 0.44        | 0/2248          |
| 49  | E     | 0.15         | 0/1657        | 0.43        | 0/2248          |
| 50  | CQ    | 0.19         | 0/1731        | 0.58        | 0/2324          |
| 50  | F     | 0.20         | 0/1731        | 0.58        | 0/2324          |
| 51  | CR    | 0.18         | 0/2096        | 0.45        | 0/2822          |
| 51  | G     | 0.37         | 1/2083 (0.0%) | 0.46        | 0/2805          |
| 52  | CS    | 0.61         | 0/1623        | 1.16        | 8/2188 (0.4%)   |
| 52  | H     | 0.16         | 0/1631        | 0.45        | 0/2199          |
| 53  | CT    | 0.19         | 0/1929        | 0.61        | 0/2571          |
| 53  | I     | 0.15         | 0/1823        | 0.44        | 0/2434          |
| 54  | CU    | 0.51         | 0/1472        | 1.13        | 4/1979 (0.2%)   |
| 54  | J     | 0.17         | 0/1490        | 0.46        | 0/2004          |
| 55  | CV    | 0.18         | 0/1606        | 0.47        | 0/2150          |
| 55  | K     | 0.15         | 0/1606        | 0.44        | 0/2150          |
| 56  | CW    | 0.15         | 0/1478        | 0.43        | 0/1978          |
| 56  | L     | 0.15         | 0/1478        | 0.45        | 0/1978          |
| 57  | CX    | 0.20         | 0/809         | 0.62        | 0/1092          |
| 57  | M     | 0.22         | 0/836         | 0.76        | 1/1130 (0.1%)   |
| 58  | CY    | 0.20         | 0/1154        | 0.51        | 2/1553 (0.1%)   |
| 58  | N     | 0.16         | 0/1175        | 0.46        | 0/1582          |
| 59  | CZ    | 0.54         | 0/921         | 1.22        | 3/1240 (0.2%)   |
| 59  | O     | 0.31         | 0/892         | 0.86        | 1/1203 (0.1%)   |
| 60  | DA    | 0.15         | 0/1210        | 0.43        | 0/1631          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 60  | P     | 0.16         | 0/1198          | 0.45        | 0/1614            |
| 61  | DB    | 0.17         | 0/915           | 0.49        | 0/1228            |
| 61  | Q     | 0.19         | 0/953           | 0.52        | 0/1279            |
| 62  | DC    | 0.49         | 0/1049          | 1.12        | 2/1409 (0.1%)     |
| 62  | R     | 0.25         | 0/1054          | 0.69        | 2/1416 (0.1%)     |
| 63  | DD    | 0.17         | 0/1103          | 0.50        | 0/1478            |
| 63  | S     | 0.23         | 0/1103          | 0.51        | 0/1478            |
| 64  | DE    | 0.20         | 0/1009          | 0.62        | 0/1354            |
| 64  | T     | 0.17         | 0/1009          | 0.50        | 0/1354            |
| 65  | DF    | 0.21         | 0/1178          | 0.53        | 0/1579            |
| 65  | U     | 0.19         | 0/1205          | 0.54        | 0/1615            |
| 66  | DG    | 0.18         | 0/1120          | 0.52        | 0/1508            |
| 66  | V     | 0.18         | 0/1120          | 0.57        | 0/1508            |
| 67  | DH    | 0.17         | 0/772           | 0.52        | 0/1045            |
| 67  | W     | 0.18         | 0/818           | 0.51        | 0/1106            |
| 68  | DI    | 0.19         | 0/683           | 0.53        | 0/918             |
| 68  | X     | 0.17         | 0/683           | 0.47        | 0/918             |
| 69  | DJ    | 0.17         | 0/1049          | 0.44        | 0/1412            |
| 69  | Y     | 0.16         | 0/1049          | 0.41        | 0/1412            |
| 70  | DK    | 0.18         | 0/1128          | 0.54        | 0/1505            |
| 70  | Z     | 0.18         | 0/1128          | 0.57        | 0/1505            |
| 71  | DL    | 0.15         | 0/1086          | 0.44        | 0/1447            |
| 71  | a     | 0.14         | 0/1100          | 0.43        | 0/1466            |
| 72  | DM    | 0.34         | 0/577           | 0.56        | 0/778             |
| 72  | b     | 0.17         | 0/585           | 0.45        | 0/789             |
| 73  | DN    | 0.15         | 0/791           | 0.51        | 0/1060            |
| 73  | c     | 0.17         | 0/782           | 0.49        | 0/1048            |
| 74  | DO    | 0.19         | 0/624           | 0.56        | 0/843             |
| 74  | d     | 0.16         | 0/624           | 0.46        | 0/843             |
| 75  | DP    | 0.21         | 0/478           | 0.65        | 0/640             |
| 75  | e     | 0.18         | 0/470           | 0.53        | 0/629             |
| 76  | DQ    | 0.23         | 0/461           | 0.57        | 0/613             |
| 76  | f     | 0.35         | 0/466           | 0.85        | 2/620 (0.3%)      |
| 77  | DR    | 0.37         | 0/478           | 0.77        | 0/637             |
| 77  | g     | 0.19         | 0/482           | 0.54        | 0/642             |
| 78  | DS    | 0.53         | 0/564           | 1.40        | 4/749 (0.5%)      |
| 78  | h     | 0.22         | 0/585           | 0.73        | 0/778             |
| 79  | AR    | 0.16         | 0/2451          | 0.46        | 0/3337            |
| 79  | DT    | 0.62         | 1/2414 (0.0%)   | 1.26        | 16/3286 (0.5%)    |
| 80  | BE    | 0.18         | 0/1696          | 0.47        | 0/2276            |
| 81  | P0    | 0.36         | 0/857           | 0.75        | 0/1148            |
| 82  | 12    | 0.40         | 0/486           | 0.76        | 2/653 (0.3%)      |
| All | All   | 0.23         | 4/427902 (0.0%) | 0.54        | 149/627694 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 51  | G     | 149 | TYR  | C-O   | -14.47 | 1.17        | 1.23     |
| 19  | y     | 60  | PRO  | CA-C  | -6.84  | 1.48        | 1.51     |
| 28  | BU    | 29  | HIS  | C-N   | -5.87  | 1.26        | 1.33     |
| 79  | DT    | 201 | LEU  | C-N   | 5.18   | 1.41        | 1.33     |

All (149) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | AU    | 102  | U    | P-O3'-C3'   | -9.29 | 106.26      | 120.20   |
| 1   | AS    | 524  | G    | P-O3'-C3'   | -8.88 | 106.89      | 120.20   |
| 46  | CM    | 72   | A    | P-O3'-C3'   | -8.84 | 106.94      | 120.20   |
| 79  | DT    | 40   | LYS  | CD-CE-NZ    | 8.66  | 139.60      | 111.90   |
| 1   | AS    | 523  | G    | P-O3'-C3'   | -8.63 | 107.25      | 120.20   |
| 46  | CM    | 75   | U    | P-O3'-C3'   | -8.51 | 107.44      | 120.20   |
| 1   | 1     | 1653 | C    | P-O3'-C3'   | -8.16 | 107.96      | 120.20   |
| 1   | 1     | 602  | A    | P-O3'-C3'   | -8.07 | 108.10      | 120.20   |
| 3   | AU    | 105  | A    | P-O3'-C3'   | -7.91 | 108.34      | 120.20   |
| 46  | CM    | 71   | A    | P-O3'-C3'   | -7.83 | 108.46      | 120.20   |
| 14  | BG    | 48   | PRO  | N-CA-CB     | -7.77 | 95.09       | 103.25   |
| 1   | 1     | 1652 | A    | P-O3'-C3'   | -7.76 | 108.56      | 120.20   |
| 1   | 1     | 3125 | U    | P-O3'-C3'   | -7.65 | 108.72      | 120.20   |
| 5   | AX    | 142  | LYS  | CB-CA-C     | -7.58 | 95.33       | 110.42   |
| 1   | 1     | 3127 | U    | O4'-C1'-N1  | 7.45  | 119.38      | 108.20   |
| 45  | i     | 38   | LYS  | CG-CD-CE    | 7.45  | 128.43      | 111.30   |
| 52  | CS    | 26   | ALA  | CA-C-N      | -7.44 | 109.21      | 122.15   |
| 52  | CS    | 26   | ALA  | C-N-CA      | -7.44 | 109.21      | 122.15   |
| 54  | CU    | 57   | PHE  | N-CA-C      | -7.43 | 97.94       | 109.76   |
| 10  | p     | 249  | LYS  | CB-CG-CD    | 7.30  | 128.10      | 111.30   |
| 1   | 1     | 1025 | G    | C5'-C4'-C3' | -7.30 | 105.06      | 116.00   |
| 1   | AS    | 646  | C    | P-O3'-C3'   | -7.23 | 109.35      | 120.20   |
| 10  | BC    | 62   | GLN  | CB-CG-CD    | 7.17  | 124.80      | 112.60   |
| 3   | AU    | 104  | A    | P-O3'-C3'   | -7.17 | 109.45      | 120.20   |
| 37  | CD    | 65   | GLU  | N-CA-C      | 7.00  | 118.80      | 111.03   |
| 76  | f     | 40   | ARG  | N-CA-C      | -6.97 | 104.78      | 113.28   |
| 1   | 1     | 3124 | U    | P-O3'-C3'   | -6.96 | 109.75      | 120.20   |
| 79  | DT    | 159  | PRO  | N-CA-C      | -6.90 | 105.08      | 113.98   |
| 20  | z     | 157  | GLU  | CB-CA-C     | -6.87 | 95.95       | 110.31   |
| 1   | AS    | 441  | U    | O5'-C5'-C4' | 6.76  | 121.84      | 111.70   |
| 3   | AU    | 103  | G    | P-O3'-C3'   | -6.69 | 110.16      | 120.20   |
| 46  | CM    | 812  | C    | P-O3'-C3'   | -6.66 | 110.22      | 120.20   |
| 46  | B     | 676  | G    | O4'-C1'-N9  | 6.58  | 118.37      | 108.50   |
| 52  | CS    | 25   | LEU  | CA-CB-CG    | 6.55  | 139.24      | 116.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 48  | CO    | 115  | ARG  | CA-CB-CG    | -6.43 | 101.24      | 114.10   |
| 52  | CS    | 27   | THR  | CA-C-N      | -6.43 | 113.30      | 122.94   |
| 52  | CS    | 27   | THR  | C-N-CA      | -6.43 | 113.30      | 122.94   |
| 46  | B     | 1283 | U    | O3'-P-O5'   | 6.40  | 113.60      | 104.00   |
| 28  | BU    | 124  | ALA  | CA-C-N      | 6.39  | 132.50      | 121.07   |
| 28  | BU    | 124  | ALA  | C-N-CA      | 6.39  | 132.50      | 121.07   |
| 46  | CM    | 278  | U    | C4'-C3'-O3' | 6.38  | 118.97      | 109.40   |
| 54  | CU    | 99   | ALA  | N-CA-C      | 6.33  | 119.19      | 107.60   |
| 28  | BU    | 57   | MET  | CA-C-N      | -6.33 | 109.16      | 121.06   |
| 28  | BU    | 57   | MET  | C-N-CA      | -6.33 | 109.16      | 121.06   |
| 45  | i     | 37   | LYS  | N-CA-C      | 6.33  | 124.28      | 110.80   |
| 59  | O     | 39   | ASP  | N-CA-C      | -6.30 | 103.59      | 111.90   |
| 54  | CU    | 70   | GLN  | CA-CB-CG    | 6.22  | 126.55      | 114.10   |
| 46  | CM    | 277  | G    | O5'-C5'-C4' | 6.21  | 120.82      | 111.50   |
| 10  | p     | 249  | LYS  | CB-CA-C     | -6.20 | 100.50      | 110.79   |
| 52  | CS    | 25   | LEU  | CB-CA-C     | 6.16  | 122.39      | 109.65   |
| 1   | AS    | 645  | A    | P-O3'-C3'   | -6.15 | 110.97      | 120.20   |
| 78  | DS    | 154  | GLY  | CA-C-N      | -6.13 | 111.75      | 121.86   |
| 78  | DS    | 154  | GLY  | C-N-CA      | -6.13 | 111.75      | 121.86   |
| 48  | CO    | 202  | GLN  | N-CA-C      | -6.10 | 104.71      | 111.36   |
| 46  | CM    | 970  | G    | O3'-P-O5'   | 6.10  | 113.15      | 104.00   |
| 22  | BO    | 122  | ASN  | N-CA-C      | 6.08  | 120.21      | 113.21   |
| 46  | CM    | 811  | U    | P-O3'-C3'   | -6.03 | 111.16      | 120.20   |
| 1   | 1     | 1218 | G    | O5'-C5'-C4' | 6.02  | 120.73      | 111.70   |
| 46  | B     | 824  | U    | P-O5'-C5'   | -6.01 | 111.89      | 120.90   |
| 1   | 1     | 599  | U    | P-O5'-C5'   | 5.97  | 129.86      | 120.90   |
| 46  | CM    | 810  | U    | P-O3'-C3'   | -5.96 | 111.25      | 120.20   |
| 59  | CZ    | 68   | GLU  | N-CA-C      | -5.94 | 98.23       | 108.56   |
| 79  | DT    | 103  | ARG  | CA-C-N      | -5.89 | 114.93      | 122.77   |
| 79  | DT    | 103  | ARG  | C-N-CA      | -5.89 | 114.93      | 122.77   |
| 1   | AS    | 1576 | A    | O4'-C1'-N9  | 5.88  | 117.32      | 108.50   |
| 22  | BO    | 125  | THR  | N-CA-C      | -5.88 | 100.32      | 109.72   |
| 46  | B     | 1744 | G    | P-O3'-C3'   | -5.86 | 111.41      | 120.20   |
| 1   | AS    | 1576 | A    | C4-N9-C1'   | 5.83  | 143.80      | 126.30   |
| 1   | 1     | 1025 | G    | O5'-C5'-C4' | 5.82  | 120.24      | 111.50   |
| 57  | M     | 89   | LEU  | N-CA-C      | -5.80 | 108.01      | 114.62   |
| 46  | CM    | 218  | A    | C5'-C4'-O4' | -5.78 | 101.13      | 109.80   |
| 46  | CM    | 217  | A    | O5'-C5'-C4' | 5.77  | 120.16      | 111.50   |
| 79  | DT    | 19   | TRP  | CA-CB-CG    | 5.76  | 124.54      | 113.60   |
| 62  | DC    | 35   | LYS  | N-CA-C      | -5.75 | 104.65      | 111.03   |
| 45  | CL    | 78   | SER  | CA-C-N      | 5.74  | 130.40      | 122.77   |
| 45  | CL    | 78   | SER  | C-N-CA      | 5.74  | 130.40      | 122.77   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 14  | t     | 131  | LYS  | N-CA-CB    | -5.72 | 101.64      | 110.56   |
| 10  | p     | 249  | LYS  | N-CA-CB    | 5.71  | 118.52      | 110.12   |
| 62  | R     | 121  | ILE  | CA-C-N     | -5.68 | 111.49      | 122.06   |
| 62  | R     | 121  | ILE  | C-N-CA     | -5.68 | 111.49      | 122.06   |
| 45  | i     | 38   | LYS  | CA-C-N     | 5.67  | 132.36      | 121.54   |
| 45  | i     | 38   | LYS  | C-N-CA     | 5.67  | 132.36      | 121.54   |
| 14  | BG    | 130  | THR  | CA-C-N     | -5.64 | 112.48      | 122.74   |
| 14  | BG    | 130  | THR  | C-N-CA     | -5.64 | 112.48      | 122.74   |
| 62  | DC    | 17   | PHE  | CA-C-O     | -5.58 | 115.05      | 121.47   |
| 43  | CJ    | 43   | TYR  | CA-CB-CG   | 5.58  | 123.95      | 113.90   |
| 48  | CO    | 187  | LYS  | CA-C-N     | 5.58  | 128.22      | 120.29   |
| 48  | CO    | 187  | LYS  | C-N-CA     | 5.58  | 128.22      | 120.29   |
| 26  | BS    | 128  | SER  | CA-C-N     | 5.55  | 129.48      | 120.60   |
| 26  | BS    | 128  | SER  | C-N-CA     | 5.55  | 129.48      | 120.60   |
| 82  | 12    | 105  | PRO  | N-CA-C     | -5.54 | 101.06      | 112.47   |
| 45  | i     | 38   | LYS  | CA-CB-CG   | 5.53  | 125.16      | 114.10   |
| 76  | f     | 39   | CYS  | CB-CA-C    | -5.51 | 99.00       | 111.30   |
| 1   | 1     | 1576 | A    | O4'-C1'-N9 | 5.50  | 116.76      | 108.50   |
| 5   | AX    | 142  | LYS  | CA-CB-CG   | 5.50  | 125.10      | 114.10   |
| 79  | DT    | 290  | ALA  | CA-C-N     | -5.49 | 113.08      | 120.82   |
| 79  | DT    | 290  | ALA  | C-N-CA     | -5.49 | 113.08      | 120.82   |
| 28  | BU    | 57   | MET  | N-CA-C     | -5.47 | 102.38      | 110.48   |
| 1   | 1     | 1576 | A    | C4-N9-C1'  | 5.46  | 142.68      | 126.30   |
| 79  | DT    | 213  | LYS  | CA-C-N     | -5.46 | 113.12      | 120.87   |
| 79  | DT    | 213  | LYS  | C-N-CA     | -5.46 | 113.12      | 120.87   |
| 52  | CS    | 156  | ARG  | CA-C-N     | -5.42 | 114.39      | 122.74   |
| 52  | CS    | 156  | ARG  | C-N-CA     | -5.42 | 114.39      | 122.74   |
| 46  | CM    | 822  | G    | O3'-P-O5'  | -5.41 | 95.89       | 104.00   |
| 59  | CZ    | 101  | ALA  | CA-C-N     | -5.40 | 110.82      | 121.41   |
| 59  | CZ    | 101  | ALA  | C-N-CA     | -5.40 | 110.82      | 121.41   |
| 46  | B     | 824  | U    | O4'-C1'-N1 | -5.39 | 100.42      | 108.50   |
| 25  | BR    | 111  | LYS  | CB-CG-CD   | 5.38  | 123.69      | 111.30   |
| 79  | DT    | 142  | MET  | CA-C-N     | -5.36 | 113.54      | 122.64   |
| 79  | DT    | 142  | MET  | C-N-CA     | -5.36 | 113.54      | 122.64   |
| 23  | BP    | 56   | ILE  | CA-CB-CG1  | -5.35 | 101.30      | 110.40   |
| 79  | DT    | 275  | PHE  | N-CA-C     | -5.34 | 101.18      | 109.72   |
| 46  | B     | 835  | A    | O5'-P-OP1  | 5.34  | 124.01      | 108.00   |
| 14  | BG    | 194  | GLU  | CA-C-N     | -5.32 | 113.20      | 120.44   |
| 14  | BG    | 194  | GLU  | C-N-CA     | -5.32 | 113.20      | 120.44   |
| 20  | z     | 157  | GLU  | CA-CB-CG   | 5.28  | 124.65      | 114.10   |
| 79  | DT    | 40   | LYS  | CG-CD-CE   | 5.26  | 123.41      | 111.30   |
| 1   | AS    | 522  | C    | P-O3'-C3'  | -5.24 | 112.34      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | CU    | 40   | LYS  | CA-CB-CG    | 5.23  | 124.57      | 114.10   |
| 26  | BS    | 38   | LEU  | CA-C-N      | -5.22 | 115.42      | 123.14   |
| 26  | BS    | 38   | LEU  | C-N-CA      | -5.22 | 115.42      | 123.14   |
| 46  | B     | 1284 | G    | P-O5'-C5'   | 5.22  | 128.72      | 120.90   |
| 14  | t     | 131  | LYS  | CD-CE-NZ    | -5.20 | 95.26       | 111.90   |
| 46  | B     | 1364 | U    | O3'-P-O5'   | 5.20  | 111.80      | 104.00   |
| 45  | CL    | 125  | ALA  | N-CA-C      | 5.17  | 116.72      | 111.14   |
| 45  | i     | 110  | SER  | N-CA-C      | -5.16 | 103.59      | 110.55   |
| 1   | AS    | 2417 | A    | C5'-C4'-C3' | -5.15 | 108.27      | 116.00   |
| 36  | CC    | 119  | LYS  | CG-CD-CE    | -5.14 | 99.47       | 111.30   |
| 14  | t     | 66   | ASN  | CB-CA-C     | -5.13 | 102.82      | 110.88   |
| 78  | DS    | 178  | LYS  | CA-C-N      | 5.12  | 131.33      | 121.54   |
| 78  | DS    | 178  | LYS  | C-N-CA      | 5.12  | 131.33      | 121.54   |
| 1   | 1     | 1218 | G    | C5'-C4'-C3' | 5.12  | 122.88      | 115.20   |
| 46  | CM    | 1672 | G    | O3'-P-O5'   | 5.12  | 111.68      | 104.00   |
| 1   | 1     | 481  | G    | C2'-C3'-O3' | -5.12 | 106.03      | 113.70   |
| 14  | BG    | 48   | PRO  | CA-N-CD     | -5.11 | 104.85      | 112.00   |
| 1   | AS    | 1563 | A    | P-O5'-C5'   | -5.11 | 113.24      | 120.90   |
| 82  | 12    | 107  | ASP  | N-CA-C      | -5.09 | 107.11      | 113.72   |
| 46  | CM    | 218  | A    | P-O3'-C3'   | -5.08 | 112.58      | 120.20   |
| 79  | DT    | 201  | LEU  | CA-C-N      | 5.07  | 128.39      | 120.68   |
| 79  | DT    | 201  | LEU  | C-N-CA      | 5.07  | 128.39      | 120.68   |
| 45  | CL    | 137  | ASP  | CA-C-N      | -5.07 | 112.17      | 122.31   |
| 45  | CL    | 137  | ASP  | C-N-CA      | -5.07 | 112.17      | 122.31   |
| 1   | 1     | 2484 | U    | N1-C1'-C2'  | 5.07  | 119.60      | 112.00   |
| 58  | CY    | 26   | LYS  | CA-C-N      | 5.04  | 131.16      | 121.54   |
| 58  | CY    | 26   | LYS  | C-N-CA      | 5.04  | 131.16      | 121.54   |
| 1   | 1     | 600  | U    | C4'-C3'-O3' | 5.03  | 120.55      | 113.00   |
| 1   | 1     | 598  | U    | O4'-C1'-N1  | 5.03  | 116.05      | 108.50   |
| 1   | AS    | 1576 | A    | C8-N9-C1'   | -5.02 | 112.65      | 127.70   |
| 79  | DT    | 176  | LYS  | N-CA-C      | 5.01  | 117.57      | 109.40   |

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   | 1     | 68791 | 0        | 34571    | 1315    | 0            |
| 1   | AS    | 66291 | 0        | 33318    | 1281    | 0            |
| 2   | 3     | 2579  | 0        | 1303     | 42      | 0            |
| 2   | AT    | 2579  | 0        | 1304     | 40      | 0            |
| 3   | 4     | 3313  | 0        | 1674     | 67      | 0            |
| 3   | AU    | 3353  | 0        | 1694     | 88      | 0            |
| 4   | AW    | 1888  | 0        | 1962     | 54      | 0            |
| 4   | j     | 1888  | 0        | 1962     | 48      | 0            |
| 5   | AX    | 3077  | 0        | 3166     | 70      | 0            |
| 5   | k     | 3077  | 0        | 3166     | 55      | 0            |
| 6   | AY    | 2734  | 0        | 2862     | 63      | 0            |
| 6   | l     | 2734  | 0        | 2862     | 64      | 0            |
| 7   | AZ    | 2394  | 0        | 2361     | 40      | 0            |
| 7   | m     | 2409  | 0        | 2372     | 45      | 0            |
| 8   | BA    | 1210  | 0        | 1285     | 28      | 0            |
| 8   | n     | 1242  | 0        | 1321     | 32      | 0            |
| 9   | BB    | 1816  | 0        | 1900     | 32      | 0            |
| 9   | o     | 1843  | 0        | 1932     | 30      | 0            |
| 10  | BC    | 1805  | 0        | 1925     | 108     | 0            |
| 10  | p     | 1825  | 0        | 1946     | 30      | 0            |
| 11  | BD    | 1519  | 0        | 1588     | 39      | 0            |
| 11  | q     | 1519  | 0        | 1588     | 27      | 0            |
| 12  | r     | 1681  | 0        | 1722     | 30      | 0            |
| 13  | BF    | 1371  | 0        | 1410     | 39      | 0            |
| 13  | s     | 1371  | 0        | 1410     | 33      | 0            |
| 14  | BG    | 1610  | 0        | 1686     | 108     | 0            |
| 14  | t     | 1610  | 0        | 1686     | 41      | 0            |
| 15  | BH    | 1029  | 0        | 1116     | 22      | 0            |
| 15  | u     | 1015  | 0        | 1098     | 28      | 0            |
| 16  | BI    | 1713  | 0        | 1764     | 61      | 0            |
| 16  | v     | 1713  | 0        | 1764     | 51      | 0            |
| 17  | BJ    | 1590  | 0        | 1705     | 21      | 0            |
| 17  | w     | 1590  | 0        | 1705     | 32      | 0            |
| 18  | BK    | 1396  | 0        | 1421     | 40      | 0            |
| 18  | x     | 1352  | 0        | 1371     | 32      | 0            |
| 19  | BL    | 1458  | 0        | 1556     | 39      | 0            |
| 19  | y     | 1458  | 0        | 1556     | 28      | 0            |
| 20  | BM    | 1457  | 0        | 1564     | 43      | 0            |
| 20  | z     | 1457  | 0        | 1564     | 38      | 0            |
| 21  | 0     | 1423  | 0        | 1480     | 40      | 0            |
| 21  | BN    | 1423  | 0        | 1480     | 33      | 0            |
| 22  | 2     | 1262  | 0        | 1314     | 18      | 0            |
| 22  | BO    | 1262  | 0        | 1314     | 34      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | 5     | 803   | 0        | 825      | 22      | 0            |
| 23  | BP    | 794   | 0        | 812      | 73      | 0            |
| 24  | 6     | 977   | 0        | 1025     | 9       | 0            |
| 24  | BQ    | 977   | 0        | 1026     | 13      | 0            |
| 25  | 7     | 945   | 0        | 1010     | 45      | 0            |
| 25  | BR    | 877   | 0        | 939      | 43      | 0            |
| 26  | 8     | 965   | 0        | 1019     | 17      | 0            |
| 26  | BS    | 960   | 0        | 1014     | 63      | 0            |
| 27  | 9     | 989   | 0        | 1064     | 31      | 0            |
| 27  | BT    | 989   | 0        | 1064     | 37      | 0            |
| 28  | AA    | 1087  | 0        | 1154     | 16      | 0            |
| 28  | BU    | 1087  | 0        | 1154     | 83      | 0            |
| 29  | AB    | 1170  | 0        | 1203     | 20      | 0            |
| 29  | BV    | 1170  | 0        | 1203     | 29      | 0            |
| 30  | AC    | 464   | 0        | 491      | 14      | 0            |
| 30  | BW    | 482   | 0        | 510      | 7       | 0            |
| 31  | AD    | 747   | 0        | 789      | 20      | 0            |
| 31  | BX    | 715   | 0        | 759      | 12      | 0            |
| 32  | AE    | 881   | 0        | 925      | 16      | 0            |
| 32  | BY    | 881   | 0        | 925      | 15      | 0            |
| 33  | AF    | 1000  | 0        | 1069     | 12      | 0            |
| 33  | BZ    | 991   | 0        | 1061     | 21      | 0            |
| 34  | AG    | 847   | 0        | 893      | 18      | 0            |
| 34  | CA    | 847   | 0        | 893      | 15      | 0            |
| 35  | AH    | 887   | 0        | 947      | 28      | 0            |
| 35  | CB    | 869   | 0        | 928      | 32      | 0            |
| 36  | AI    | 963   | 0        | 1059     | 34      | 0            |
| 36  | CC    | 974   | 0        | 1071     | 71      | 0            |
| 37  | AJ    | 758   | 0        | 838      | 11      | 0            |
| 37  | CD    | 736   | 0        | 812      | 42      | 0            |
| 38  | AK    | 677   | 0        | 697      | 20      | 0            |
| 38  | CE    | 677   | 0        | 697      | 26      | 0            |
| 39  | AL    | 617   | 0        | 675      | 7       | 0            |
| 39  | CF    | 617   | 0        | 675      | 45      | 0            |
| 40  | AM    | 438   | 0        | 475      | 9       | 0            |
| 40  | CG    | 438   | 0        | 475      | 13      | 0            |
| 41  | AN    | 402   | 0        | 435      | 7       | 0            |
| 41  | CH    | 403   | 0        | 437      | 9       | 0            |
| 42  | AO    | 236   | 0        | 285      | 6       | 0            |
| 42  | CI    | 227   | 0        | 272      | 8       | 0            |
| 43  | AP    | 828   | 0        | 894      | 17      | 0            |
| 43  | CJ    | 828   | 0        | 893      | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | AQ    | 698   | 0        | 734      | 12      | 0            |
| 44  | CK    | 698   | 0        | 734      | 15      | 0            |
| 45  | CL    | 919   | 0        | 899      | 66      | 0            |
| 45  | i     | 805   | 0        | 782      | 78      | 0            |
| 46  | B     | 36410 | 0        | 18322    | 910     | 0            |
| 46  | CM    | 36839 | 0        | 18535    | 963     | 0            |
| 47  | C     | 1627  | 0        | 1644     | 48      | 0            |
| 47  | CN    | 1627  | 0        | 1644     | 41      | 0            |
| 48  | CO    | 1717  | 0        | 1796     | 180     | 0            |
| 48  | D     | 1724  | 0        | 1805     | 35      | 0            |
| 49  | CP    | 1629  | 0        | 1728     | 31      | 0            |
| 49  | E     | 1629  | 0        | 1728     | 36      | 0            |
| 50  | CQ    | 1707  | 0        | 1807     | 64      | 0            |
| 50  | F     | 1707  | 0        | 1807     | 67      | 0            |
| 51  | CR    | 2055  | 0        | 2137     | 55      | 0            |
| 51  | G     | 2042  | 0        | 2126     | 60      | 0            |
| 52  | CS    | 1606  | 0        | 1677     | 111     | 0            |
| 52  | H     | 1614  | 0        | 1688     | 43      | 0            |
| 53  | CT    | 1904  | 0        | 1994     | 80      | 0            |
| 53  | I     | 1798  | 0        | 1874     | 56      | 0            |
| 54  | CU    | 1449  | 0        | 1546     | 144     | 0            |
| 54  | J     | 1466  | 0        | 1561     | 47      | 0            |
| 55  | CV    | 1579  | 0        | 1602     | 43      | 0            |
| 55  | K     | 1579  | 0        | 1602     | 42      | 0            |
| 56  | CW    | 1453  | 0        | 1532     | 34      | 0            |
| 56  | L     | 1453  | 0        | 1532     | 37      | 0            |
| 57  | CX    | 791   | 0        | 805      | 45      | 0            |
| 57  | M     | 817   | 0        | 828      | 50      | 0            |
| 58  | CY    | 1129  | 0        | 1183     | 20      | 0            |
| 58  | N     | 1150  | 0        | 1201     | 26      | 0            |
| 59  | CZ    | 913   | 0        | 934      | 103     | 0            |
| 59  | O     | 885   | 0        | 915      | 50      | 0            |
| 60  | DA    | 1187  | 0        | 1249     | 18      | 0            |
| 60  | P     | 1175  | 0        | 1235     | 31      | 0            |
| 61  | DB    | 905   | 0        | 947      | 38      | 0            |
| 61  | Q     | 942   | 0        | 981      | 21      | 0            |
| 62  | DC    | 1029  | 0        | 1078     | 98      | 0            |
| 62  | R     | 1034  | 0        | 1083     | 51      | 0            |
| 63  | DD    | 1085  | 0        | 1150     | 38      | 0            |
| 63  | S     | 1085  | 0        | 1150     | 54      | 0            |
| 64  | DE    | 997   | 0        | 1053     | 45      | 0            |
| 64  | T     | 997   | 0        | 1053     | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 65  | DF    | 1161  | 0        | 1205     | 46      | 0            |
| 65  | U     | 1187  | 0        | 1237     | 35      | 0            |
| 66  | DG    | 1100  | 0        | 1114     | 34      | 0            |
| 66  | V     | 1100  | 0        | 1114     | 33      | 0            |
| 67  | DH    | 763   | 0        | 824      | 22      | 0            |
| 67  | W     | 808   | 0        | 871      | 27      | 0            |
| 68  | DI    | 676   | 0        | 677      | 18      | 0            |
| 68  | X     | 676   | 0        | 677      | 19      | 0            |
| 69  | DJ    | 1032  | 0        | 1066     | 33      | 0            |
| 69  | Y     | 1032  | 0        | 1066     | 25      | 0            |
| 70  | DK    | 1110  | 0        | 1182     | 34      | 0            |
| 70  | Z     | 1110  | 0        | 1182     | 31      | 0            |
| 71  | DL    | 1072  | 0        | 1123     | 26      | 0            |
| 71  | a     | 1086  | 0        | 1132     | 24      | 0            |
| 72  | DM    | 570   | 0        | 609      | 19      | 0            |
| 72  | b     | 578   | 0        | 613      | 14      | 0            |
| 73  | DN    | 779   | 0        | 833      | 25      | 0            |
| 73  | c     | 770   | 0        | 824      | 17      | 0            |
| 74  | DO    | 614   | 0        | 630      | 9       | 0            |
| 74  | d     | 614   | 0        | 627      | 10      | 0            |
| 75  | DP    | 476   | 0        | 510      | 26      | 0            |
| 75  | e     | 468   | 0        | 499      | 12      | 0            |
| 76  | DQ    | 449   | 0        | 426      | 14      | 0            |
| 76  | f     | 454   | 0        | 430      | 18      | 0            |
| 77  | DR    | 470   | 0        | 512      | 26      | 0            |
| 77  | g     | 474   | 0        | 515      | 16      | 0            |
| 78  | DS    | 555   | 0        | 585      | 61      | 0            |
| 78  | h     | 574   | 0        | 606      | 30      | 0            |
| 79  | AR    | 2398  | 0        | 2374     | 75      | 0            |
| 79  | DT    | 2362  | 0        | 2335     | 332     | 0            |
| 80  | BE    | 1662  | 0        | 1709     | 28      | 0            |
| 81  | P0    | 845   | 0        | 884      | 94      | 0            |
| 82  | 12    | 480   | 0        | 477      | 54      | 0            |
| 83  | 1     | 57    | 0        | 52       | 6       | 0            |
| 83  | AS    | 57    | 0        | 52       | 7       | 0            |
| 84  | 0     | 4     | 0        | 0        | 0       | 0            |
| 84  | 1     | 469   | 0        | 0        | 0       | 0            |
| 84  | 2     | 1     | 0        | 0        | 0       | 0            |
| 84  | 3     | 7     | 0        | 0        | 0       | 0            |
| 84  | 4     | 1     | 0        | 0        | 0       | 0            |
| 84  | 6     | 1     | 0        | 0        | 0       | 0            |
| 84  | AB    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 84  | AC    | 1     | 0        | 0        | 0       | 0            |
| 84  | AD    | 1     | 0        | 0        | 0       | 0            |
| 84  | AJ    | 1     | 0        | 0        | 0       | 0            |
| 84  | AP    | 2     | 0        | 0        | 0       | 0            |
| 84  | AS    | 389   | 0        | 0        | 0       | 0            |
| 84  | AT    | 5     | 0        | 0        | 0       | 0            |
| 84  | AU    | 5     | 0        | 0        | 0       | 0            |
| 84  | AW    | 1     | 0        | 0        | 0       | 0            |
| 84  | AX    | 3     | 0        | 0        | 0       | 0            |
| 84  | AY    | 2     | 0        | 0        | 0       | 0            |
| 84  | AZ    | 1     | 0        | 0        | 0       | 0            |
| 84  | B     | 99    | 0        | 0        | 0       | 0            |
| 84  | BB    | 2     | 0        | 0        | 0       | 0            |
| 84  | BC    | 1     | 0        | 0        | 0       | 0            |
| 84  | BE    | 1     | 0        | 0        | 0       | 0            |
| 84  | BI    | 1     | 0        | 0        | 0       | 0            |
| 84  | BK    | 1     | 0        | 0        | 0       | 0            |
| 84  | BL    | 2     | 0        | 0        | 0       | 0            |
| 84  | BO    | 1     | 0        | 0        | 0       | 0            |
| 84  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 84  | BZ    | 1     | 0        | 0        | 0       | 0            |
| 84  | C     | 1     | 0        | 0        | 0       | 0            |
| 84  | CA    | 1     | 0        | 0        | 0       | 0            |
| 84  | CB    | 1     | 0        | 0        | 0       | 0            |
| 84  | CG    | 1     | 0        | 0        | 0       | 0            |
| 84  | CL    | 2     | 0        | 0        | 0       | 0            |
| 84  | CM    | 78    | 0        | 0        | 0       | 0            |
| 84  | CW    | 1     | 0        | 0        | 0       | 0            |
| 84  | D     | 1     | 0        | 0        | 0       | 0            |
| 84  | DA    | 1     | 0        | 0        | 0       | 0            |
| 84  | DG    | 1     | 0        | 0        | 0       | 0            |
| 84  | DH    | 1     | 0        | 0        | 0       | 0            |
| 84  | DK    | 2     | 0        | 0        | 0       | 0            |
| 84  | E     | 1     | 0        | 0        | 0       | 0            |
| 84  | F     | 1     | 0        | 0        | 0       | 0            |
| 84  | G     | 1     | 0        | 0        | 0       | 0            |
| 84  | K     | 1     | 0        | 0        | 0       | 0            |
| 84  | L     | 1     | 0        | 0        | 0       | 0            |
| 84  | P0    | 1     | 0        | 0        | 1       | 0            |
| 84  | Q     | 2     | 0        | 0        | 0       | 0            |
| 84  | R     | 4     | 0        | 0        | 0       | 0            |
| 84  | T     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 84  | Y     | 2      | 0        | 0        | 0       | 0            |
| 84  | a     | 1      | 0        | 0        | 0       | 0            |
| 84  | j     | 1      | 0        | 0        | 0       | 0            |
| 84  | k     | 3      | 0        | 0        | 0       | 0            |
| 84  | m     | 1      | 0        | 0        | 0       | 0            |
| 84  | o     | 4      | 0        | 0        | 0       | 0            |
| 84  | r     | 1      | 0        | 0        | 0       | 0            |
| 84  | u     | 1      | 0        | 0        | 0       | 0            |
| 84  | v     | 2      | 0        | 0        | 0       | 0            |
| 84  | w     | 1      | 0        | 0        | 0       | 0            |
| 84  | x     | 1      | 0        | 0        | 0       | 0            |
| 84  | y     | 3      | 0        | 0        | 0       | 0            |
| 85  | AH    | 1      | 0        | 0        | 0       | 0            |
| 85  | AK    | 1      | 0        | 0        | 0       | 0            |
| 85  | AN    | 1      | 0        | 0        | 0       | 0            |
| 85  | AP    | 1      | 0        | 0        | 0       | 0            |
| 85  | AQ    | 1      | 0        | 0        | 0       | 0            |
| 85  | CB    | 1      | 0        | 0        | 0       | 0            |
| 85  | CE    | 1      | 0        | 0        | 0       | 0            |
| 85  | CH    | 1      | 0        | 0        | 0       | 0            |
| 85  | CJ    | 1      | 0        | 0        | 0       | 0            |
| 85  | CK    | 1      | 0        | 0        | 0       | 0            |
| 85  | DN    | 1      | 0        | 0        | 0       | 0            |
| 85  | DQ    | 1      | 0        | 0        | 0       | 0            |
| 85  | DS    | 1      | 0        | 0        | 0       | 0            |
| 85  | c     | 1      | 0        | 0        | 0       | 0            |
| 85  | d     | 1      | 0        | 0        | 0       | 0            |
| 85  | f     | 1      | 0        | 0        | 0       | 0            |
| 85  | h     | 1      | 0        | 0        | 0       | 0            |
| 86  | B     | 34     | 0        | 40       | 6       | 0            |
| 86  | CM    | 34     | 0        | 40       | 5       | 0            |
| All | All   | 400037 | 0        | 297473   | 8914    | 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 13.

All (8914) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 78:DS:162:GLU:HA  | 78:DS:173:PHE:HA | 1.29                     | 1.14              |
| 79:DT:226:LYS:HD2 | 79:DT:227:THR:H  | 1.14                     | 1.11              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:BM:176:ARG:HH12 | 20:BM:180:LYS:HB2  | 1.17                     | 1.03              |
| 79:DT:126:ALA:HB2  | 79:DT:155:VAL:HG13 | 1.40                     | 1.03              |
| 10:BC:62:GLN:HG3   | 16:BI:28:TRP:CH2   | 1.95                     | 1.02              |
| 46:CM:694:C:H3'    | 46:CM:695:C:H5''   | 1.40                     | 1.01              |
| 25:BR:102:LYS:HE3  | 25:BR:105:ARG:NH2  | 1.73                     | 1.01              |
| 79:DT:40:LYS:HZ3   | 79:DT:67:HIS:HA    | 1.26                     | 1.00              |
| 10:BC:62:GLN:HG3   | 16:BI:28:TRP:CZ2   | 1.95                     | 1.00              |
| 81:P0:50:VAL:HB    | 81:P0:88:PHE:HB2   | 1.44                     | 0.99              |
| 59:O:36:LEU:C      | 59:O:38:HIS:H      | 1.70                     | 0.99              |
| 45:i:64:LEU:HD21   | 62:R:120:SER:HA    | 1.45                     | 0.99              |
| 2:AT:85:G:H1'      | 9:BB:218:GLN:HE21  | 1.27                     | 0.98              |
| 1:AS:447:U:H2'     | 1:AS:448:U:H5''    | 1.43                     | 0.97              |
| 46:CM:697:U:H3     | 46:CM:724:G:H1     | 1.13                     | 0.97              |
| 79:DT:313:MET:HG3  | 79:DT:314:THR:H    | 1.29                     | 0.96              |
| 35:CB:58:ARG:HD3   | 35:CB:59:PRO:HD2   | 1.49                     | 0.95              |
| 79:DT:110:ASP:HB2  | 79:DT:128:ARG:HD2  | 1.47                     | 0.95              |
| 46:B:853:G:H1      | 46:B:945:U:H3      | 1.14                     | 0.95              |
| 62:R:10:ARG:HG2    | 62:R:13:LYS:HB3    | 1.45                     | 0.94              |
| 50:F:65:ARG:HD2    | 57:M:91:ARG:HH11   | 1.32                     | 0.94              |
| 23:BP:19:VAL:HB    | 23:BP:62:ASN:HB2   | 1.50                     | 0.94              |
| 45:CL:132:GLU:HG3  | 50:CQ:95:ARG:HG3   | 1.47                     | 0.94              |
| 1:1:3199:G:H1      | 1:1:3218:U:H3      | 1.15                     | 0.94              |
| 1:AS:538:G:H1      | 1:AS:547:U:H3      | 0.94                     | 0.94              |
| 25:BR:96:GLN:HG3   | 25:BR:99:SER:HB2   | 1.46                     | 0.94              |
| 46:CM:484:G:H1     | 46:CM:499:U:H3     | 1.12                     | 0.93              |
| 10:BC:62:GLN:CG    | 16:BI:28:TRP:CZ2   | 2.51                     | 0.93              |
| 69:DJ:2:THR:HG22   | 69:DJ:3:ARG:H      | 1.33                     | 0.93              |
| 52:CS:27:THR:HG22  | 52:CS:28:THR:H     | 1.31                     | 0.93              |
| 52:CS:200:ASN:HB2  | 52:CS:208:SER:HB3  | 1.51                     | 0.92              |
| 1:AS:3199:G:H1     | 1:AS:3218:U:H3     | 1.09                     | 0.92              |
| 57:M:17:GLN:H      | 57:M:88:PRO:HB3    | 1.34                     | 0.92              |
| 1:AS:1870:A:N7     | 20:BM:20:ARG:NH2   | 2.18                     | 0.92              |
| 79:DT:206:SER:HB2  | 79:DT:223:ASN:HD22 | 1.33                     | 0.92              |
| 46:CM:853:G:H1     | 46:CM:945:U:H3     | 1.17                     | 0.92              |
| 79:DT:12:THR:HG23  | 79:DT:53:ASN:CG    | 1.94                     | 0.91              |
| 1:AS:564:G:H2'     | 1:AS:565:A:C8      | 2.05                     | 0.91              |
| 48:CO:66:PHE:CE2   | 61:DB:29:SER:HB2   | 2.06                     | 0.91              |
| 46:B:1198:G:H1     | 46:B:1436:U:H3     | 1.04                     | 0.91              |
| 59:CZ:36:LEU:HB2   | 59:CZ:41:LEU:HG    | 1.53                     | 0.91              |
| 54:CU:5:ILE:HG21   | 54:CU:10:PRO:HG3   | 1.51                     | 0.91              |
| 1:1:1233:G:H1      | 1:1:1247:A:H61     | 1.20                     | 0.90              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:DT:201:LEU:HD23 | 79:DT:201:LEU:H    | 1.33                     | 0.90              |
| 46:B:653:G:HO2'    | 46:B:672:U:H3      | 0.95                     | 0.90              |
| 46:B:671:G:H3'     | 46:B:672:U:H5'     | 1.53                     | 0.90              |
| 55:K:191:GLU:HB3   | 58:N:23:PRO:HG3    | 1.54                     | 0.90              |
| 1:AS:2194:G:H1     | 1:AS:2207:A:H61    | 1.16                     | 0.90              |
| 46:CM:1067:C:H4'   | 68:DI:58:TYR:HE1   | 1.37                     | 0.90              |
| 78:DS:127:TYR:HD1  | 78:DS:128:THR:HG23 | 1.35                     | 0.90              |
| 1:AS:437:G:H22     | 1:AS:620:A:H61     | 1.11                     | 0.89              |
| 54:CU:122:LEU:HD11 | 54:CU:169:TYR:CD1  | 2.06                     | 0.89              |
| 59:CZ:132:GLU:HA   | 59:CZ:136:LEU:HD12 | 1.51                     | 0.89              |
| 1:1:3313:G:H1      | 1:1:3322:U:H3      | 1.18                     | 0.89              |
| 82:12:103:ASN:HA   | 82:12:144:ASP:HA   | 1.55                     | 0.89              |
| 1:AS:1556:G:N7     | 26:BS:36:LYS:NZ    | 2.21                     | 0.88              |
| 35:AH:58:ARG:HD3   | 35:AH:59:PRO:HD2   | 1.55                     | 0.88              |
| 52:CS:53:VAL:HB    | 52:CS:59:VAL:HG22  | 1.55                     | 0.88              |
| 45:i:64:LEU:HD13   | 62:R:121:ILE:HG13  | 1.55                     | 0.88              |
| 26:BS:66:PRO:HG2   | 36:CC:36:LEU:HD11  | 1.54                     | 0.88              |
| 25:BR:82:ILE:HG12  | 53:CT:131:LYS:HD2  | 1.56                     | 0.88              |
| 82:12:104:ILE:HD11 | 82:12:142:ARG:HB2  | 1.54                     | 0.88              |
| 46:B:1395:G:N2     | 46:B:1398:G:OP2    | 2.07                     | 0.88              |
| 55:K:120:THR:HG21  | 55:K:133:ALA:HA    | 1.56                     | 0.88              |
| 1:AS:3313:G:H1     | 1:AS:3322:U:H3     | 1.20                     | 0.88              |
| 65:U:140:THR:HA    | 65:U:143:ARG:HH21  | 1.39                     | 0.88              |
| 51:CR:11:ARG:HH12  | 51:CR:24:SER:HB2   | 1.38                     | 0.88              |
| 54:CU:30:LEU:HD12  | 54:CU:34:LEU:HD21  | 1.56                     | 0.88              |
| 28:BU:134:LEU:HG   | 28:BU:135:HIS:H    | 1.39                     | 0.87              |
| 46:CM:1670:U:H3    | 46:CM:1705:G:H1    | 1.23                     | 0.87              |
| 46:CM:1742:A:HO2'  | 46:CM:1743:A:H8    | 0.89                     | 0.87              |
| 46:CM:1236:U:O2'   | 46:CM:1237:C:O2    | 1.93                     | 0.86              |
| 46:CM:1230:G:H1    | 46:CM:1235:U:H3    | 1.18                     | 0.86              |
| 48:CO:59:ASP:OD1   | 48:CO:60:GLY:N     | 2.08                     | 0.86              |
| 79:DT:13:LEU:N     | 79:DT:307:ILE:O    | 2.07                     | 0.86              |
| 39:CF:40:GLN:HB2   | 39:CF:57:ASN:HA    | 1.58                     | 0.86              |
| 81:P0:15:LEU:HG    | 81:P0:63:ILE:HD11  | 1.57                     | 0.86              |
| 52:H:95:ASN:OD1    | 52:H:107:LYS:NZ    | 2.09                     | 0.86              |
| 20:BM:155:LEU:HA   | 20:BM:158:GLU:OE1  | 1.76                     | 0.86              |
| 62:DC:36:LEU:HD23  | 62:DC:36:LEU:H     | 1.38                     | 0.86              |
| 79:DT:46:LYS:HB3   | 79:DT:57:ILE:HG22  | 1.58                     | 0.86              |
| 79:DT:243:SER:HB3  | 79:DT:248:TRP:H    | 1.41                     | 0.85              |
| 1:1:3141:U:H3      | 1:1:3245:A:H62     | 1.24                     | 0.85              |
| 67:DH:26:THR:HG22  | 67:DH:87:LYS:HG3   | 1.59                     | 0.85              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:CO:28:ASP:OD1  | 48:CO:29:TRP:N     | 2.10                     | 0.85              |
| 79:DT:169:ALA:HB3 | 79:DT:199:ILE:HD11 | 1.59                     | 0.85              |
| 50:CQ:215:GLU:HG3 | 50:CQ:216:ASP:H    | 1.42                     | 0.84              |
| 22:BO:112:ASN:HB3 | 22:BO:128:LEU:HD13 | 1.57                     | 0.84              |
| 46:CM:79:C:OP1    | 53:CT:159:ARG:NH2  | 2.10                     | 0.84              |
| 46:CM:538:G:N2    | 77:DR:25:GLU:OE2   | 2.10                     | 0.84              |
| 51:CR:45:VAL:HG23 | 51:CR:61:VAL:HG11  | 1.59                     | 0.84              |
| 45:CL:135:GLU:OE1 | 50:CQ:95:ARG:NH2   | 2.10                     | 0.84              |
| 46:CM:1529:G:N2   | 46:CM:1556:A:OP2   | 2.11                     | 0.84              |
| 45:i:113:ARG:HH21 | 50:F:117:ARG:HB2   | 1.43                     | 0.84              |
| 57:M:88:PRO:HD2   | 57:M:91:ARG:HB2    | 1.59                     | 0.84              |
| 3:AU:135:G:H5'    | 26:BS:49:LYS:HD3   | 1.57                     | 0.84              |
| 79:DT:13:LEU:HB2  | 79:DT:307:ILE:HB   | 1.59                     | 0.84              |
| 54:J:25:GLU:HG3   | 54:J:35:ARG:HH12   | 1.42                     | 0.83              |
| 1:1:496:A:H4'     | 8:n:27:GLN:HG3     | 1.60                     | 0.83              |
| 1:AS:2334:A:N3    | 18:BK:131:ARG:NH2  | 2.25                     | 0.83              |
| 37:CD:73:LYS:HE3  | 37:CD:79:HIS:HB2   | 1.59                     | 0.83              |
| 1:AS:1542:A:N7    | 16:BI:71:ARG:NH1   | 2.27                     | 0.83              |
| 10:BC:221:ALA:HA  | 10:BC:225:GLU:HB2  | 1.59                     | 0.83              |
| 46:CM:1410:A:H2'  | 49:CP:87:ALA:HB3   | 1.60                     | 0.83              |
| 26:8:75:LYS:HB3   | 26:8:81:THR:HG23   | 1.58                     | 0.83              |
| 48:CO:128:LYS:HE2 | 48:CO:132:ASP:HA   | 1.60                     | 0.83              |
| 48:CO:24:PHE:HD1  | 48:CO:27:LYS:HE2   | 1.42                     | 0.83              |
| 78:DS:127:TYR:CD1 | 78:DS:128:THR:HG23 | 2.14                     | 0.83              |
| 46:B:217:A:N6     | 46:B:828:U:O2      | 2.12                     | 0.83              |
| 1:AS:1014:G:N2    | 1:AS:1030:U:O2     | 2.09                     | 0.83              |
| 27:BT:39:LEU:HD22 | 27:BT:43:TYR:HE2   | 1.44                     | 0.83              |
| 48:CO:179:CYS:HB2 | 48:CO:183:GLN:HB2  | 1.58                     | 0.82              |
| 1:AS:1384:U:OP1   | 33:BZ:105:LYS:NZ   | 2.13                     | 0.82              |
| 1:1:171:G:H1      | 1:1:246:U:H3       | 1.26                     | 0.82              |
| 1:AS:1561:U:O2'   | 1:AS:1562:G:OP1    | 1.97                     | 0.82              |
| 26:BS:115:ARG:HD3 | 26:BS:121:LYS:HE3  | 1.61                     | 0.82              |
| 1:1:3235:A:N7     | 8:n:45:ARG:NH1     | 2.28                     | 0.82              |
| 46:B:442:C:OP1    | 71:a:102:LYS:NZ    | 2.11                     | 0.82              |
| 46:CM:78:A:H8     | 53:CT:154:ARG:HG3  | 1.44                     | 0.82              |
| 1:1:1018:U:O2'    | 1:1:1019:U:H5'     | 1.79                     | 0.82              |
| 18:BK:50:GLN:OE1  | 18:BK:56:ARG:NH2   | 2.12                     | 0.82              |
| 79:DT:226:LYS:HD2 | 79:DT:227:THR:N    | 1.92                     | 0.82              |
| 1:AS:12:A:H4'     | 26:BS:39:LYS:HD2   | 1.59                     | 0.82              |
| 37:CD:59:LEU:HG   | 37:CD:68:ALA:HB2   | 1.61                     | 0.82              |
| 47:CN:200:ASP:HB2 | 64:DE:85:VAL:HG23  | 1.62                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:CO:81:TYR:HB2   | 48:CO:109:LYS:HD3  | 1.61                     | 0.82              |
| 1:AS:1562:G:N2     | 1:AS:1564:U:O4     | 2.13                     | 0.82              |
| 79:DT:112:LEU:HD23 | 79:DT:153:SER:HA   | 1.60                     | 0.82              |
| 1:AS:3165:U:C2     | 1:AS:3166:A:H1'    | 2.15                     | 0.82              |
| 28:BU:127:ASN:O    | 28:BU:129:TRP:N    | 2.13                     | 0.82              |
| 46:CM:95:G:OP1     | 51:CR:6:LYS:NZ     | 2.13                     | 0.82              |
| 82:12:146:LYS:HD2  | 82:12:151:ILE:HG23 | 1.62                     | 0.82              |
| 82:12:162:VAL:HG12 | 82:12:164:GLU:HG2  | 1.62                     | 0.82              |
| 1:AS:1091:U:H4'    | 1:AS:1092:U:H5'    | 1.61                     | 0.81              |
| 28:BU:56:LYS:O     | 28:BU:56:LYS:HD3   | 1.80                     | 0.81              |
| 28:BU:107:ARG:O    | 28:BU:111:LYS:HG3  | 1.80                     | 0.81              |
| 67:DH:21:ILE:HG12  | 67:DH:117:ILE:HG12 | 1.61                     | 0.81              |
| 46:B:1236:U:O2'    | 46:B:1237:C:O2     | 1.97                     | 0.81              |
| 51:G:104:ASP:HB3   | 51:G:110:ALA:HB2   | 1.61                     | 0.81              |
| 46:CM:458:A:HO2'   | 51:CR:27:TYR:HH    | 1.26                     | 0.81              |
| 52:CS:54:LYS:HG3   | 52:CS:138:VAL:HG21 | 1.62                     | 0.81              |
| 54:J:48:ASN:OD1    | 54:J:167:GLN:NE2   | 2.13                     | 0.81              |
| 79:DT:194:GLY:H    | 79:DT:214:ASP:HB3  | 1.44                     | 0.81              |
| 1:AS:2420:G:H1     | 1:AS:2483:U:H3     | 1.28                     | 0.81              |
| 14:BG:169:TYR:O    | 14:BG:173:ARG:HG2  | 1.80                     | 0.81              |
| 46:B:1334:G:N3     | 46:B:1365:C:N4     | 2.27                     | 0.81              |
| 54:CU:34:LEU:HD11  | 54:CU:69:VAL:HG11  | 1.61                     | 0.81              |
| 1:1:185:U:H3       | 1:1:229:C:H42      | 1.29                     | 0.81              |
| 6:1:359:GLU:O      | 21:0:26:ARG:NH1    | 2.13                     | 0.81              |
| 30:AC:58:ARG:CG    | 30:AC:59:ALA:H     | 1.93                     | 0.81              |
| 48:CO:131:ASP:OD1  | 48:CO:181:LEU:N    | 2.14                     | 0.81              |
| 81:P0:45:LEU:HD22  | 81:P0:48:ASP:OD2   | 1.81                     | 0.81              |
| 22:BO:49:GLN:HA    | 22:BO:52:MET:HE3   | 1.62                     | 0.81              |
| 48:CO:190:PRO:HG2  | 48:CO:192:VAL:HG23 | 1.63                     | 0.81              |
| 52:CS:164:PRO:HA   | 52:CS:167:ARG:HD3  | 1.63                     | 0.81              |
| 69:DJ:11:LEU:HD11  | 69:DJ:37:PHE:HE2   | 1.46                     | 0.81              |
| 79:DT:21:THR:H     | 79:DT:37:SER:HA    | 1.45                     | 0.81              |
| 46:B:216:A:N6      | 46:B:829:A:O2'     | 2.14                     | 0.80              |
| 46:B:1375:C:O5'    | 64:T:48:ASN:ND2    | 2.14                     | 0.80              |
| 54:CU:42:ILE:HG12  | 54:CU:56:VAL:HA    | 1.64                     | 0.80              |
| 79:DT:218:ILE:HG23 | 79:DT:230:THR:HG22 | 1.62                     | 0.80              |
| 1:1:653:C:H2'      | 1:1:654:A:H8       | 1.44                     | 0.80              |
| 52:CS:39:GLU:OE2   | 52:CS:41:LYS:HG2   | 1.81                     | 0.80              |
| 79:DT:288:SER:O    | 79:DT:301:GLY:N    | 2.14                     | 0.80              |
| 46:B:509:A:OP2     | 56:L:176:ASN:ND2   | 2.12                     | 0.80              |
| 46:B:512:G:H1      | 46:B:541:C:H5      | 1.27                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:M:5:LYS:HZ2     | 59:O:38:HIS:CG     | 2.00                     | 0.80              |
| 46:CM:821:U:H2'    | 46:CM:822:G:C8     | 2.16                     | 0.80              |
| 48:CO:162:ARG:HG2  | 48:CO:165:ARG:HH21 | 1.47                     | 0.80              |
| 62:DC:20:VAL:HG21  | 62:DC:36:LEU:HD13  | 1.62                     | 0.80              |
| 69:DJ:88:ARG:O     | 69:DJ:92:ASN:ND2   | 2.15                     | 0.80              |
| 20:Z:171:GLU:OE2   | 20:Z:175:GLN:NE2   | 2.14                     | 0.80              |
| 27:9:45:VAL:HG12   | 27:9:46:LYS:H      | 1.45                     | 0.80              |
| 36:CC:5:LYS:O      | 36:CC:9:LEU:HD12   | 1.82                     | 0.80              |
| 60:DA:55:ARG:NH2   | 74:DO:51:GLN:OE1   | 2.15                     | 0.80              |
| 59:O:35:SER:OG     | 59:O:41:LEU:HB2    | 1.82                     | 0.80              |
| 1:AS:3162:U:H3     | 1:AS:3166:A:H2     | 1.27                     | 0.80              |
| 1:1:581:A:H5''     | 34:AG:106:ASN:HD21 | 1.46                     | 0.80              |
| 10:BC:204:VAL:HG21 | 10:BC:212:LEU:HD13 | 1.63                     | 0.80              |
| 59:CZ:61:VAL:HG22  | 59:CZ:121:VAL:HG12 | 1.64                     | 0.80              |
| 69:DJ:37:PHE:HE1   | 69:DJ:103:ILE:HG13 | 1.46                     | 0.80              |
| 46:B:766:U:H4'     | 46:B:767:G:H5''    | 1.64                     | 0.79              |
| 81:P0:8:LYS:NZ     | 81:P0:58:MET:SD    | 2.53                     | 0.79              |
| 66:V:117:SER:HB2   | 66:V:123:ARG:HB2   | 1.64                     | 0.79              |
| 1:AS:21:G:H5''     | 38:CE:43:LYS:HG2   | 1.64                     | 0.79              |
| 25:BR:102:LYS:HE3  | 25:BR:105:ARG:HH21 | 1.42                     | 0.79              |
| 26:BS:73:MET:HG3   | 26:BS:142:ILE:HD13 | 1.64                     | 0.79              |
| 54:CU:94:ILE:HD13  | 54:CU:114:LEU:HD12 | 1.64                     | 0.79              |
| 48:CO:29:TRP:HE3   | 48:CO:45:LYS:HD3   | 1.47                     | 0.79              |
| 79:DT:93:TRP:HA    | 79:DT:100:THR:HA   | 1.64                     | 0.79              |
| 46:B:871:U:OP1     | 48:D:214:LYS:NZ    | 2.14                     | 0.79              |
| 1:AS:353:G:O6      | 38:CE:55:ARG:NH2   | 2.15                     | 0.79              |
| 10:p:247:ILE:HA    | 10:p:250:LYS:HE2   | 1.65                     | 0.79              |
| 45:i:53:LYS:HE2    | 45:i:55:LYS:HD3    | 1.65                     | 0.79              |
| 39:CF:8:ILE:HD12   | 39:CF:65:LEU:HD21  | 1.65                     | 0.79              |
| 78:DS:168:CYS:HB2  | 78:DS:172:ILE:HG21 | 1.64                     | 0.79              |
| 81:P0:5:ARG:HA     | 81:P0:8:LYS:HB2    | 1.65                     | 0.79              |
| 1:1:1481:G:N2      | 35:AH:4:ARG:HD2    | 1.97                     | 0.79              |
| 1:AS:835:C:H4'     | 1:AS:1720:U:H2'    | 1.64                     | 0.79              |
| 13:BF:7:ASN:OD1    | 13:BF:10:ARG:HG3   | 1.82                     | 0.79              |
| 23:BP:86:TYR:O     | 23:BP:90:ASN:ND2   | 2.14                     | 0.79              |
| 46:CM:1230:G:N2    | 46:CM:1235:U:O4    | 2.16                     | 0.79              |
| 30:BW:8:THR:HG22   | 30:BW:10:HIS:H     | 1.48                     | 0.79              |
| 46:CM:1042:U:H3'   | 46:CM:1043:U:H2'   | 1.65                     | 0.78              |
| 65:DF:49:LYS:NZ    | 65:DF:80:LYS:O     | 2.15                     | 0.78              |
| 79:DT:11:GLY:O     | 79:DT:309:VAL:N    | 2.17                     | 0.78              |
| 57:M:77:ARG:NH1    | 57:M:83:PRO:O      | 2.16                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:2:A:OP1      | 49:CP:171:LYS:NZ   | 2.16                     | 0.78              |
| 46:B:671:G:H5''    | 46:B:672:U:H6      | 1.49                     | 0.78              |
| 45:CL:160:LEU:O    | 45:CL:163:GLN:HG2  | 1.84                     | 0.78              |
| 65:DF:115:ARG:HG2  | 65:DF:118:LYS:HE2  | 1.66                     | 0.78              |
| 56:L:34:TYR:HA     | 56:L:122:ILE:HD13  | 1.66                     | 0.78              |
| 13:BF:85:LYS:HG2   | 62:DC:12:PHE:CE1   | 2.19                     | 0.78              |
| 46:B:352:C:H5''    | 55:K:16:ALA:HB2    | 1.66                     | 0.78              |
| 32:BY:45:THR:HG21  | 32:BY:89:PHE:HA    | 1.65                     | 0.78              |
| 47:C:124:THR:HG22  | 47:C:174:TRP:HE1   | 1.47                     | 0.78              |
| 46:CM:849:U:OP1    | 69:DJ:28:ARG:NH1   | 2.17                     | 0.78              |
| 1:AS:2545:C:O2'    | 1:AS:2547:G:N3     | 2.16                     | 0.78              |
| 1:AS:2936:G:N2     | 1:AS:2939:A:OP2    | 2.16                     | 0.78              |
| 81:P0:2:GLY:O      | 81:P0:5:ARG:NH1    | 2.16                     | 0.78              |
| 1:AS:617:A:H5'     | 1:AS:619:A:H1'     | 1.65                     | 0.77              |
| 46:B:136:U:O2'     | 53:I:149:LYS:NZ    | 2.16                     | 0.77              |
| 23:BP:28:PHE:CE1   | 23:BP:33:TYR:HB2   | 2.18                     | 0.77              |
| 46:CM:78:A:C8      | 53:CT:154:ARG:HG3  | 2.18                     | 0.77              |
| 81:P0:25:ILE:HG22  | 81:P0:26:PHE:H     | 1.49                     | 0.77              |
| 45:CL:155:LEU:HD13 | 57:CX:92:LEU:HD13  | 1.65                     | 0.77              |
| 1:AS:2516:U:O2'    | 1:AS:2519:A:N1     | 2.16                     | 0.77              |
| 46:CM:1156:A:H2'   | 46:CM:1157:G:C8    | 2.19                     | 0.77              |
| 48:CO:194:GLY:O    | 48:CO:198:GLU:HG3  | 1.83                     | 0.77              |
| 62:DC:28:MET:HE3   | 62:DC:32:GLU:HB3   | 1.64                     | 0.77              |
| 23:5:19:VAL:HG23   | 23:5:20:ALA:H      | 1.49                     | 0.77              |
| 56:CW:31:ALA:HB2   | 56:CW:42:ILE:HD11  | 1.67                     | 0.77              |
| 62:DC:15:PHE:HB3   | 62:DC:22:LEU:HB2   | 1.67                     | 0.77              |
| 1:1:1481:G:H21     | 35:AH:4:ARG:HD2    | 1.50                     | 0.77              |
| 1:1:2200:A:H2'     | 1:1:2201:A:C8      | 2.20                     | 0.77              |
| 45:i:71:LYS:O      | 45:i:73:VAL:N      | 2.14                     | 0.77              |
| 1:AS:1657:G:H2'    | 1:AS:1658:G:C8     | 2.20                     | 0.77              |
| 54:CU:74:THR:HG23  | 54:CU:86:VAL:HB    | 1.66                     | 0.77              |
| 46:B:1282:G:N2     | 46:B:1285:A:OP2    | 2.18                     | 0.77              |
| 79:DT:57:ILE:HG13  | 79:DT:58:PRO:HD2   | 1.65                     | 0.77              |
| 1:1:3157:A:OP1     | 11:q:23:ARG:NH1    | 2.17                     | 0.77              |
| 53:I:159:ARG:NH1   | 53:I:170:THR:OG1   | 2.17                     | 0.77              |
| 63:S:38:VAL:HG12   | 63:S:44:ARG:HG3    | 1.67                     | 0.77              |
| 46:CM:820:U:H2'    | 46:CM:821:U:C6     | 2.21                     | 0.76              |
| 46:CM:1152:G:H21   | 63:DD:138:GLN:HE22 | 1.31                     | 0.76              |
| 46:CM:1198:G:H1    | 46:CM:1436:U:H3    | 1.30                     | 0.76              |
| 48:CO:66:PHE:HE2   | 61:DB:29:SER:HB2   | 1.46                     | 0.76              |
| 79:DT:219:LEU:HB3  | 79:DT:228:LEU:HD23 | 1.67                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:n:45:ARG:HH12    | 18:x:178:SER:HB3   | 1.50                     | 0.76              |
| 51:G:11:ARG:HH12   | 51:G:24:SER:HB3    | 1.50                     | 0.76              |
| 30:AC:56:LYS:O     | 30:AC:58:ARG:NH1   | 2.17                     | 0.76              |
| 46:B:122:U:H2'     | 46:B:123:G:H5''    | 1.68                     | 0.76              |
| 46:B:218:A:OP2     | 46:B:817:U:H5'     | 1.84                     | 0.76              |
| 1:AS:831:G:O2'     | 1:AS:853:G:N2      | 2.17                     | 0.76              |
| 1:AS:2191:A:H2'    | 1:AS:2192:A:C8     | 2.20                     | 0.76              |
| 48:CO:36:THR:HA    | 48:CO:41:ARG:HD3   | 1.67                     | 0.76              |
| 82:12:103:ASN:HA   | 82:12:144:ASP:CA   | 2.14                     | 0.76              |
| 18:x:50:GLN:OE1    | 18:x:56:ARG:NH2    | 2.16                     | 0.76              |
| 30:AC:8:THR:HG22   | 30:AC:10:HIS:H     | 1.49                     | 0.76              |
| 46:B:1665:C:OP1    | 55:K:59:ARG:NH2    | 2.17                     | 0.76              |
| 59:O:36:LEU:C      | 59:O:38:HIS:N      | 2.31                     | 0.76              |
| 36:CC:74:LYS:HE2   | 36:CC:75:TYR:CZ    | 2.21                     | 0.76              |
| 79:DT:40:LYS:HZ3   | 79:DT:67:HIS:CA    | 1.99                     | 0.76              |
| 1:1:1091:U:H4'     | 1:1:1092:U:H5'     | 1.66                     | 0.76              |
| 46:B:1276:G:H1     | 46:B:1309:G:H22    | 1.30                     | 0.76              |
| 46:CM:948:A:OP2    | 60:DA:70:LYS:NZ    | 2.19                     | 0.76              |
| 46:CM:1742:A:O2'   | 46:CM:1743:A:H8    | 1.69                     | 0.76              |
| 59:CZ:69:GLU:O     | 59:CZ:71:ILE:N     | 2.18                     | 0.76              |
| 1:1:831:G:O2'      | 1:1:853:G:N2       | 2.18                     | 0.76              |
| 45:i:70:ASN:ND2    | 45:i:72:ASP:OD1    | 2.18                     | 0.76              |
| 1:AS:2601:U:O4     | 22:BO:2:GLY:N      | 2.17                     | 0.76              |
| 79:DT:169:ALA:HB2  | 79:DT:175:VAL:HG22 | 1.68                     | 0.76              |
| 35:CB:107:GLU:OE1  | 35:CB:107:GLU:N    | 2.18                     | 0.76              |
| 36:CC:44:ILE:O     | 36:CC:48:ARG:HG3   | 1.85                     | 0.76              |
| 46:CM:824:U:OP2    | 58:CY:28:ASN:HB2   | 1.86                     | 0.76              |
| 48:CO:143:THR:HG22 | 48:CO:205:PHE:HE2  | 1.51                     | 0.76              |
| 54:CU:71:THR:HB    | 54:CU:127:PHE:CE2  | 2.21                     | 0.76              |
| 23:BP:19:VAL:HA    | 23:BP:108:LEU:HD13 | 1.65                     | 0.76              |
| 48:CO:133:TYR:CE2  | 48:CO:181:LEU:HD22 | 2.21                     | 0.76              |
| 1:1:3087:C:O2      | 1:1:3089:C:N4      | 2.20                     | 0.75              |
| 46:B:139:U:OP1     | 53:I:149:LYS:NZ    | 2.19                     | 0.75              |
| 46:B:1042:U:H3'    | 46:B:1043:U:H2'    | 1.67                     | 0.75              |
| 10:BC:90:GLN:HB2   | 10:BC:215:LEU:HD21 | 1.66                     | 0.75              |
| 10:BC:150:LYS:O    | 10:BC:177:PRO:HD2  | 1.86                     | 0.75              |
| 1:1:1217:A:C2      | 81:P0:12:PHE:HE2   | 2.05                     | 0.75              |
| 1:1:1657:G:H2'     | 1:1:1658:G:C8      | 2.21                     | 0.75              |
| 1:AS:2558:G:O2'    | 10:BC:242:LYS:NZ   | 2.16                     | 0.75              |
| 1:AS:3318:G:H5''   | 1:AS:3319:U:H4'    | 1.66                     | 0.75              |
| 14:BG:48:PRO:HG2   | 14:BG:135:VAL:O    | 1.86                     | 0.75              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:CM:784:U:H2'    | 46:CM:785:G:H8    | 1.50                     | 0.75              |
| 62:DC:41:VAL:HG12  | 62:DC:45:PHE:CE2  | 2.20                     | 0.75              |
| 1:1:2650:A:H2      | 45:i:52:LYS:HD2   | 1.51                     | 0.75              |
| 46:B:553:A:N3      | 46:B:588:C:O2'    | 2.19                     | 0.75              |
| 46:B:653:G:N2      | 46:B:654:G:O6     | 2.19                     | 0.75              |
| 1:AS:2655:U:H2'    | 1:AS:2656:C:C6    | 2.21                     | 0.75              |
| 6:AY:300:VAL:HB    | 19:BL:39:ARG:HG2  | 1.67                     | 0.75              |
| 1:1:653:C:H2'      | 1:1:654:A:C8      | 2.21                     | 0.75              |
| 1:1:2086:C:H1'     | 1:1:3309:A:C8     | 2.21                     | 0.75              |
| 28:BU:62:VAL:O     | 28:BU:66:THR:HG23 | 1.86                     | 0.75              |
| 46:B:79:C:OP1      | 53:I:159:ARG:NH2  | 2.19                     | 0.75              |
| 10:BC:34:ASN:ND2   | 10:BC:39:GLN:HE21 | 1.85                     | 0.75              |
| 1:1:2936:G:N2      | 1:1:2939:A:OP2    | 2.18                     | 0.75              |
| 46:B:1218:G:H1     | 46:B:1237:C:H5    | 1.30                     | 0.75              |
| 50:F:138:VAL:HG22  | 50:F:152:LYS:HG2  | 1.69                     | 0.75              |
| 46:CM:738:A:OP1    | 51:CR:187:ARG:N   | 2.18                     | 0.75              |
| 46:CM:1395:G:N2    | 46:CM:1398:G:OP2  | 2.20                     | 0.75              |
| 1:AS:653:C:H2'     | 1:AS:654:A:H8     | 1.50                     | 0.75              |
| 20:BM:176:ARG:NH1  | 20:BM:176:ARG:O   | 2.17                     | 0.75              |
| 28:BU:27:LYS:HG2   | 28:BU:29:HIS:HE2  | 1.52                     | 0.75              |
| 54:CU:41:SER:O     | 54:CU:57:PHE:N    | 2.18                     | 0.75              |
| 1:AS:437:G:N2      | 1:AS:620:A:H61    | 1.83                     | 0.75              |
| 10:BC:108:GLU:O    | 10:BC:112:LYS:HG3 | 1.86                     | 0.75              |
| 52:CS:220:VAL:O    | 52:CS:224:ASN:ND2 | 2.20                     | 0.75              |
| 45:i:116:GLU:HA    | 45:i:119:VAL:HG22 | 1.68                     | 0.74              |
| 51:CR:71:GLN:HB3   | 51:CR:91:THR:HB   | 1.66                     | 0.74              |
| 1:1:359:U:OP1      | 38:AK:11:ARG:NH1  | 2.19                     | 0.74              |
| 32:AE:45:THR:HG21  | 32:AE:89:PHE:HA   | 1.69                     | 0.74              |
| 46:B:813:U:H2'     | 46:B:814:A:C8     | 2.22                     | 0.74              |
| 46:B:1431:G:N2     | 78:h:129:THR:O    | 2.19                     | 0.74              |
| 39:CF:31:VAL:HG22  | 39:CF:33:ALA:H    | 1.50                     | 0.74              |
| 41:CH:22:LYS:HG3   | 41:CH:42:THR:HG21 | 1.67                     | 0.74              |
| 79:DT:277:VAL:HG13 | 79:DT:278:GLY:H   | 1.52                     | 0.74              |
| 25:BR:111:LYS:HA   | 25:BR:114:GLU:HG2 | 1.70                     | 0.74              |
| 79:DT:88:ARG:CZ    | 79:DT:109:GLY:HA2 | 2.18                     | 0.74              |
| 1:1:1188:C:N4      | 1:1:1297:A:O2'    | 2.21                     | 0.74              |
| 46:CM:869:A:H62    | 46:CM:913:U:H3    | 1.35                     | 0.74              |
| 48:CO:180:THR:N    | 48:CO:183:GLN:OE1 | 2.20                     | 0.74              |
| 1:1:1560:U:H3      | 1:1:1571:G:H1     | 1.36                     | 0.74              |
| 46:B:1026:G:H2'    | 46:B:1027:G:C8    | 2.22                     | 0.74              |
| 50:CQ:48:GLU:HG2   | 50:CQ:88:TYR:HE2  | 1.51                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:DS:161:ARG:O    | 78:DS:174:MET:HG2  | 1.87                     | 0.74              |
| 79:DT:221:ASP:HB2  | 79:DT:228:LEU:HD13 | 1.70                     | 0.74              |
| 1:1:1631:G:N2      | 1:1:1634:A:OP2     | 2.17                     | 0.74              |
| 10:BC:117:ILE:HG12 | 10:BC:123:ALA:HB1  | 1.68                     | 0.74              |
| 46:CM:139:U:OP1    | 53:CT:149:LYS:NZ   | 2.20                     | 0.74              |
| 59:CZ:73:LYS:HG3   | 78:DS:150:VAL:HG21 | 1.69                     | 0.74              |
| 1:1:628:A:H2'      | 1:1:629:A:C8       | 2.22                     | 0.74              |
| 3:AU:94:C:OP1      | 38:CE:75:LYS:NZ    | 2.19                     | 0.74              |
| 5:AX:211:GLN:NE2   | 5:AX:283:TYR:O     | 2.21                     | 0.74              |
| 20:BM:176:ARG:HG2  | 46:CM:838:G:OP1    | 1.87                     | 0.74              |
| 46:CM:72:A:H2'     | 46:CM:73:U:H4'     | 1.70                     | 0.74              |
| 1:1:3179:U:OP2     | 15:u:121:ARG:NH2   | 2.20                     | 0.74              |
| 46:B:1419:G:O2'    | 76:f:24:CYS:SG     | 2.46                     | 0.74              |
| 59:O:40:GLY:HA2    | 59:O:124:LYS:HG2   | 1.70                     | 0.74              |
| 37:CD:61:ARG:HH21  | 37:CD:93:ILE:HG23  | 1.53                     | 0.74              |
| 48:CO:23:PRO:O     | 48:CO:27:LYS:NZ    | 2.18                     | 0.74              |
| 46:B:1512:A:H5'    | 66:V:93:HIS:HB2    | 1.70                     | 0.74              |
| 48:D:128:LYS:HG2   | 48:D:134:VAL:HG22  | 1.69                     | 0.74              |
| 1:AS:429:U:H2'     | 1:AS:430:G:H8      | 1.53                     | 0.74              |
| 1:1:654:A:H2'      | 1:1:655:A:C8       | 2.23                     | 0.73              |
| 52:H:29:ILE:HB     | 52:H:34:GLN:HE21   | 1.50                     | 0.73              |
| 1:AS:1761:U:C5     | 20:BM:43:LYS:HE3   | 2.23                     | 0.73              |
| 48:CO:168:MET:O    | 48:CO:172:MET:HG3  | 1.88                     | 0.73              |
| 63:S:37:LEU:HD22   | 66:V:10:PRO:HG3    | 1.69                     | 0.73              |
| 24:BQ:80:ARG:NH1   | 24:BQ:97:ASP:OD1   | 2.21                     | 0.73              |
| 65:DF:69:ILE:HG22  | 65:DF:73:MET:HE2   | 1.69                     | 0.73              |
| 42:AO:7:LYS:NZ     | 46:B:1761:G:OP1    | 2.21                     | 0.73              |
| 46:B:593:G:H5'     | 56:L:40:ARG:HH22   | 1.53                     | 0.73              |
| 62:R:81:ARG:HB2    | 62:R:117:GLY:HA3   | 1.70                     | 0.73              |
| 10:BC:62:GLN:HG2   | 16:BI:28:TRP:CZ2   | 2.23                     | 0.73              |
| 14:BG:155:GLU:OE1  | 14:BG:159:ARG:NH2  | 2.17                     | 0.73              |
| 46:B:1487:C:OP1    | 66:V:122:ARG:NH2   | 2.21                     | 0.73              |
| 1:AS:1678:U:O2     | 23:BP:85:LYS:HG2   | 1.88                     | 0.73              |
| 1:AS:1713:U:H2'    | 1:AS:1714:G:C8     | 2.23                     | 0.73              |
| 54:CU:160:TYR:HE2  | 54:CU:161:LYS:HZ3  | 1.36                     | 0.73              |
| 67:DH:41:ILE:HD11  | 67:DH:54:PRO:HD3   | 1.69                     | 0.73              |
| 1:1:2191:A:H2'     | 1:1:2192:A:C8      | 2.23                     | 0.73              |
| 46:B:1019:C:HO2'   | 69:Y:2:THR:N       | 1.85                     | 0.73              |
| 28:BU:87:LEU:HD12  | 28:BU:88:ASP:H     | 1.54                     | 0.73              |
| 46:CM:695:C:O2'    | 46:CM:696:U:OP1    | 2.07                     | 0.73              |
| 46:B:1460:G:H2'    | 46:B:1461:A:H8     | 1.52                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BX:57:GLU:HB2  | 35:CB:94:LEU:HD11  | 1.69                     | 0.73              |
| 59:CZ:103:LEU:O   | 59:CZ:105:GLN:NE2  | 2.21                     | 0.73              |
| 1:AS:1870:A:OP1   | 20:BM:18:GLY:N     | 2.20                     | 0.73              |
| 14:BG:122:LYS:HB3 | 36:CC:119:LYS:H    | 1.53                     | 0.73              |
| 54:CU:40:LYS:NZ   | 54:CU:58:VAL:O     | 2.21                     | 0.73              |
| 70:DK:107:PHE:HD2 | 70:DK:114:LYS:HD3  | 1.52                     | 0.73              |
| 1:1:1662:G:H2'    | 1:1:1663:A:H8      | 1.53                     | 0.73              |
| 1:1:2395:U:H5''   | 4:j:221:LYS:HE3    | 1.69                     | 0.73              |
| 3:4:150:G:OP1     | 26:8:27:ARG:NH2    | 2.21                     | 0.73              |
| 6:l:42:ARG:HD2    | 6:l:114:VAL:HG22   | 1.71                     | 0.73              |
| 50:F:65:ARG:HD2   | 57:M:91:ARG:NH1    | 2.03                     | 0.73              |
| 75:e:8:THR:HG21   | 75:e:59:SER:HB2    | 1.69                     | 0.73              |
| 79:DT:117:ALA:HA  | 79:DT:157:ILE:HD12 | 1.69                     | 0.73              |
| 46:B:693:U:H4'    | 54:J:96:PRO:HG3    | 1.71                     | 0.73              |
| 65:U:92:GLN:OE1   | 65:U:115:ARG:NH2   | 2.22                     | 0.73              |
| 1:AS:437:G:H22    | 1:AS:620:A:N6      | 1.85                     | 0.73              |
| 1:1:2530:C:N4     | 31:AD:59:GLU:OE2   | 2.20                     | 0.73              |
| 46:B:948:A:N7     | 60:P:70:LYS:NZ     | 2.36                     | 0.73              |
| 1:AS:1760:U:OP1   | 20:BM:43:LYS:HE2   | 1.89                     | 0.73              |
| 10:BC:71:LYS:HG2  | 10:BC:234:TRP:CE3  | 2.24                     | 0.73              |
| 45:CL:40:ASP:O    | 45:CL:42:ALA:N     | 2.21                     | 0.73              |
| 51:CR:152:PRO:HG3 | 53:CT:212:LEU:HD23 | 1.71                     | 0.73              |
| 79:DT:40:LYS:NZ   | 79:DT:67:HIS:HA    | 2.02                     | 0.73              |
| 45:i:104:GLN:HA   | 45:i:109:GLN:HE22  | 1.54                     | 0.72              |
| 46:B:540:A:N6     | 77:g:25:GLU:OE2    | 2.22                     | 0.72              |
| 46:B:814:A:O2'    | 46:B:815:U:OP2     | 2.05                     | 0.72              |
| 26:BS:86:VAL:HG11 | 26:BS:95:ILE:HD11  | 1.70                     | 0.72              |
| 28:BU:42:ILE:HG13 | 28:BU:74:LEU:HD12  | 1.71                     | 0.72              |
| 31:BX:24:LYS:HB2  | 31:BX:96:ASP:HB3   | 1.70                     | 0.72              |
| 36:CC:6:THR:O     | 36:CC:10:ARG:HG3   | 1.87                     | 0.72              |
| 46:CM:1238:U:H5'' | 78:DS:172:ILE:HG23 | 1.69                     | 0.72              |
| 77:DR:49:LEU:HD22 | 77:DR:54:ARG:HG2   | 1.71                     | 0.72              |
| 1:1:169:G:N2      | 1:1:248:U:O2       | 2.20                     | 0.72              |
| 1:1:564:G:H2'     | 1:1:565:A:C8       | 2.24                     | 0.72              |
| 35:AH:81:CYS:SG   | 35:AH:82:ALA:N     | 2.62                     | 0.72              |
| 72:b:67:ASP:O     | 72:b:70:LYS:NZ     | 2.22                     | 0.72              |
| 1:AS:2194:G:H1    | 1:AS:2207:A:N6     | 1.87                     | 0.72              |
| 1:1:2504:C:OP1    | 4:j:37:ARG:NH2     | 2.21                     | 0.72              |
| 45:i:107:TRP:HA   | 50:F:116:ILE:HD11  | 1.71                     | 0.72              |
| 22:BO:142:SER:OG  | 22:BO:144:GLU:OE1  | 2.07                     | 0.72              |
| 48:CO:97:LEU:HB2  | 48:CO:232:HIS:CE1  | 2.23                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:DM:78:VAL:HG12  | 72:DM:81:ARG:HH21  | 1.54                     | 0.72              |
| 79:DT:179:ASP:HB2  | 79:DT:186:ASN:HD21 | 1.54                     | 0.72              |
| 1:1:2334:A:N3      | 18:x:131:ARG:NH2   | 2.35                     | 0.72              |
| 48:CO:131:ASP:HB3  | 48:CO:180:THR:HG22 | 1.70                     | 0.72              |
| 79:DT:82:LEU:HD21  | 79:DT:104:PHE:HE2  | 1.55                     | 0.72              |
| 46:B:1205:C:O3'    | 57:M:52:LYS:NZ     | 2.22                     | 0.72              |
| 50:CQ:124:LEU:HD11 | 50:CQ:153:TYR:HB3  | 1.71                     | 0.72              |
| 1:1:3207:G:OP1     | 17:w:160:LYS:NZ    | 2.16                     | 0.72              |
| 63:S:86:LYS:HG2    | 63:S:116:LEU:HD13  | 1.72                     | 0.72              |
| 46:CM:399:A:H1'    | 51:CR:3:ARG:HH21   | 1.52                     | 0.72              |
| 1:1:1892:A:H61     | 1:1:2317:C:H42     | 1.38                     | 0.72              |
| 13:s:101:ASN:HD22  | 13:s:130:VAL:HA    | 1.55                     | 0.72              |
| 53:I:159:ARG:HB2   | 53:I:170:THR:HB    | 1.70                     | 0.72              |
| 1:AS:169:G:N2      | 1:AS:248:U:O2      | 2.21                     | 0.72              |
| 46:CM:1511:A:H2'   | 46:CM:1512:A:C8    | 2.23                     | 0.72              |
| 49:CP:177:PRO:HD3  | 56:CW:17:ARG:HH22  | 1.55                     | 0.72              |
| 52:CS:27:THR:HG22  | 52:CS:28:THR:N     | 2.04                     | 0.72              |
| 82:12:112:ILE:HG22 | 82:12:132:ILE:HD13 | 1.69                     | 0.72              |
| 6:l:290:LEU:HD22   | 19:y:129:LEU:HD11  | 1.70                     | 0.72              |
| 46:B:876:A:H2'     | 46:B:877:G:H8      | 1.55                     | 0.72              |
| 46:B:1156:A:H2'    | 46:B:1157:G:C8     | 2.25                     | 0.72              |
| 46:B:1546:G:C5     | 65:U:134:ARG:HD3   | 2.24                     | 0.72              |
| 51:G:45:VAL:HG23   | 51:G:61:VAL:HG11   | 1.70                     | 0.72              |
| 63:S:12:LYS:HG3    | 63:S:13:LYS:H      | 1.54                     | 0.72              |
| 1:AS:627:U:H2'     | 1:AS:628:A:C8      | 2.25                     | 0.72              |
| 1:AS:683:G:OP2     | 14:BG:35:ARG:NH1   | 2.23                     | 0.72              |
| 1:AS:1626:U:OP1    | 28:BU:67:LYS:NZ    | 2.13                     | 0.72              |
| 36:CC:21:LEU:O     | 36:CC:25:LYS:HG3   | 1.89                     | 0.72              |
| 45:CL:82:LYS:HD3   | 46:CM:1163:G:H4'   | 1.72                     | 0.72              |
| 46:CM:476:A:OP1    | 77:DR:37:ARG:NH1   | 2.23                     | 0.72              |
| 82:12:104:ILE:CD1  | 82:12:142:ARG:HB2  | 2.19                     | 0.72              |
| 1:AS:62:A:H5''     | 16:BI:174:ILE:HG21 | 1.71                     | 0.72              |
| 1:AS:2086:C:H1'    | 1:AS:3309:A:C8     | 2.25                     | 0.72              |
| 46:B:583:A:OP1     | 77:g:15:LYS:NZ     | 2.23                     | 0.72              |
| 62:R:41:VAL:HG13   | 62:R:84:ILE:HD13   | 1.71                     | 0.72              |
| 1:1:2130:A:HO2'    | 1:1:2221:A:HO2'    | 1.36                     | 0.71              |
| 5:AX:152:LYS:HG2   | 5:AX:189:SER:HA    | 1.72                     | 0.71              |
| 73:DN:74:CYS:SG    | 73:DN:75:VAL:N     | 2.63                     | 0.71              |
| 1:1:2420:G:H1      | 1:1:2483:U:H3      | 1.38                     | 0.71              |
| 79:AR:16:HIS:CE1   | 79:AR:37:SER:HB2   | 2.25                     | 0.71              |
| 1:AS:1059:G:N7     | 1:AS:1093:G:O2'    | 2.23                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:1093:G:H4'    | 22:BO:129:LYS:HG2  | 1.72                     | 0.71              |
| 46:CM:766:U:H4'    | 46:CM:767:G:H5''   | 1.70                     | 0.71              |
| 48:CO:90:GLU:OE2   | 48:CO:97:LEU:N     | 2.22                     | 0.71              |
| 1:1:662:U:H2'      | 1:1:663:A:C8       | 2.24                     | 0.71              |
| 18:x:122:ALA:HB3   | 18:x:143:PRO:HB2   | 1.71                     | 0.71              |
| 46:B:1127:A:H5''   | 73:c:2:PRO:HB3     | 1.70                     | 0.71              |
| 46:B:1485:G:H4'    | 66:V:121:GLY:H     | 1.55                     | 0.71              |
| 47:C:63:ILE:HG12   | 68:X:36:ILE:HG12   | 1.69                     | 0.71              |
| 10:BC:89:ALA:O     | 10:BC:93:LYS:HG3   | 1.89                     | 0.71              |
| 46:CM:1468:C:H5''  | 46:CM:1508:G:H22   | 1.55                     | 0.71              |
| 50:CQ:128:MET:HE2  | 50:CQ:135:VAL:HG12 | 1.72                     | 0.71              |
| 1:AS:3161:U:H2'    | 1:AS:3162:U:C6     | 2.26                     | 0.71              |
| 79:DT:256:GLY:HA3  | 79:DT:270:GLU:HG2  | 1.72                     | 0.71              |
| 82:12:112:ILE:HA   | 82:12:115:LYS:HB2  | 1.72                     | 0.71              |
| 11:q:22:ALA:O      | 11:q:39:LYS:NZ     | 2.23                     | 0.71              |
| 1:AS:65:A:OP2      | 14:BG:100:ARG:NH1  | 2.23                     | 0.71              |
| 54:CU:63:LEU:HD11  | 54:CU:67:ARG:HH21  | 1.54                     | 0.71              |
| 81:P0:45:LEU:HA    | 81:P0:48:ASP:HB3   | 1.72                     | 0.71              |
| 1:1:2655:U:H2'     | 1:1:2656:C:C6      | 2.25                     | 0.71              |
| 53:I:135:PRO:HB2   | 53:I:141:ILE:HG12  | 1.73                     | 0.71              |
| 1:AS:308:A:H5''    | 37:CD:79:HIS:CD2   | 2.25                     | 0.71              |
| 10:BC:101:GLU:OE2  | 10:BC:106:LYS:HA   | 1.91                     | 0.71              |
| 26:BS:135:ILE:HA   | 26:BS:138:ARG:HD3  | 1.71                     | 0.71              |
| 35:CB:107:GLU:O    | 35:CB:111:LYS:NZ   | 2.17                     | 0.71              |
| 46:CM:1485:G:N2    | 46:CM:1496:C:O2    | 2.19                     | 0.71              |
| 1:AS:269:G:H5''    | 16:BI:14:LYS:HE2   | 1.72                     | 0.71              |
| 1:AS:786:U:H5''    | 6:AY:113:LYS:HD3   | 1.73                     | 0.71              |
| 1:AS:2836:A:H5''   | 80:BE:114:GLY:HA2  | 1.72                     | 0.71              |
| 59:CZ:41:LEU:HA    | 59:CZ:122:VAL:O    | 1.90                     | 0.71              |
| 46:B:1579:A:H2'    | 46:B:1580:A:H8     | 1.56                     | 0.71              |
| 46:B:1753:A:N1     | 73:c:80:HIS:ND1    | 2.39                     | 0.71              |
| 1:AS:628:A:H2'     | 1:AS:629:A:C8      | 2.25                     | 0.71              |
| 10:BC:158:VAL:HG23 | 10:BC:161:ILE:HD12 | 1.71                     | 0.71              |
| 47:C:124:THR:O     | 47:C:164:ASN:ND2   | 2.23                     | 0.71              |
| 46:CM:1410:A:H2'   | 49:CP:87:ALA:CB    | 2.21                     | 0.71              |
| 1:1:3287:A:H2'     | 1:1:3288:A:C8      | 2.26                     | 0.71              |
| 49:E:138:TYR:O     | 69:Y:98:GLN:NE2    | 2.22                     | 0.71              |
| 62:R:10:ARG:CG     | 62:R:13:LYS:HB3    | 2.18                     | 0.71              |
| 62:R:98:ASN:HB2    | 62:R:121:ILE:O     | 1.91                     | 0.71              |
| 48:CO:219:LYS:NZ   | 48:CO:220:GLN:O    | 2.20                     | 0.71              |
| 79:DT:46:LYS:HG3   | 79:DT:59:LYS:CE    | 2.20                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:2155:G:OP2    | 4:j:128:ARG:NH1    | 2.24                     | 0.70              |
| 46:B:859:C:OP1    | 48:D:159:SER:OG    | 2.08                     | 0.70              |
| 14:BG:47:ALA:O    | 14:BG:49:ARG:N     | 2.24                     | 0.70              |
| 26:BS:62:ILE:HD13 | 26:BS:94:GLN:HB3   | 1.72                     | 0.70              |
| 48:CO:227:SER:O   | 48:CO:231:LEU:HG   | 1.91                     | 0.70              |
| 1:1:1400:G:N2     | 1:1:1403:A:OP2     | 2.19                     | 0.70              |
| 17:w:2:SER:N      | 21:0:161:LYS:HZ3   | 1.89                     | 0.70              |
| 1:AS:1115:C:H2'   | 1:AS:1116:A:H8     | 1.55                     | 0.70              |
| 1:AS:1663:A:H2'   | 1:AS:1664:G:C8     | 2.26                     | 0.70              |
| 10:BC:179:ALA:HB2 | 10:BC:219:ILE:HD13 | 1.73                     | 0.70              |
| 31:BX:42:LYS:HB3  | 31:BX:103:LEU:HD21 | 1.72                     | 0.70              |
| 50:CQ:166:ARG:NH2 | 76:DQ:54:LYS:O     | 2.24                     | 0.70              |
| 1:1:1233:G:H21    | 82:12:138:SER:HB2  | 1.56                     | 0.70              |
| 20:z:165:ARG:HD2  | 46:B:835:A:H5'     | 1.72                     | 0.70              |
| 31:AD:46:ILE:HG21 | 31:AD:55:LYS:HG3   | 1.73                     | 0.70              |
| 46:B:1324:C:O2'   | 46:B:1326:A:N7     | 2.24                     | 0.70              |
| 47:C:35:PRO:O     | 47:C:52:LYS:NZ     | 2.24                     | 0.70              |
| 13:BF:85:LYS:HG2  | 62:DC:12:PHE:CD1   | 2.27                     | 0.70              |
| 75:DP:12:VAL:HG22 | 75:DP:52:ASP:H     | 1.55                     | 0.70              |
| 79:DT:50:GLY:H    | 79:DT:55:TYR:HA    | 1.56                     | 0.70              |
| 79:DT:88:ARG:NH1  | 79:DT:110:ASP:OD1  | 2.24                     | 0.70              |
| 46:B:92:A:OP1     | 51:G:7:LYS:NZ      | 2.25                     | 0.70              |
| 1:AS:3233:A:OP1   | 8:BA:45:ARG:NH2    | 2.22                     | 0.70              |
| 10:BC:62:GLN:NE2  | 10:BC:66:LEU:HB2   | 2.06                     | 0.70              |
| 23:BP:43:VAL:N    | 23:BP:46:ILE:O     | 2.21                     | 0.70              |
| 46:CM:690:C:H2'   | 46:CM:691:U:C6     | 2.25                     | 0.70              |
| 79:DT:243:SER:OG  | 79:DT:245:ASN:O    | 2.08                     | 0.70              |
| 46:B:856:G:H2'    | 46:B:857:G:C8      | 2.26                     | 0.70              |
| 46:B:1300:U:OP1   | 46:B:1313:G:N2     | 2.22                     | 0.70              |
| 46:B:1511:A:H2'   | 46:B:1512:A:C8     | 2.25                     | 0.70              |
| 46:CM:1241:A:H5'  | 46:CM:1242:U:C6    | 2.27                     | 0.70              |
| 46:CM:1460:G:H2'  | 46:CM:1461:A:H8    | 1.55                     | 0.70              |
| 62:DC:81:ARG:NH1  | 62:DC:97:TYR:O     | 2.24                     | 0.70              |
| 14:BG:16:LYS:O    | 14:BG:18:TRP:N     | 2.25                     | 0.70              |
| 1:1:694:C:OP2     | 6:l:120:ARG:NH2    | 2.25                     | 0.70              |
| 6:l:113:LYS:NZ    | 16:v:204:SER:OG    | 2.24                     | 0.70              |
| 1:AS:976:A:H2'    | 1:AS:977:U:H5'     | 1.73                     | 0.70              |
| 1:AS:1094:A:OP2   | 22:BO:130:ARG:NH1  | 2.24                     | 0.70              |
| 18:BK:122:ALA:HB3 | 18:BK:143:PRO:HB2  | 1.73                     | 0.70              |
| 46:CM:784:U:H2'   | 46:CM:785:G:C8     | 2.25                     | 0.70              |
| 46:CM:1387:A:OP1  | 64:DE:56:HIS:NE2   | 2.23                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:CQ:219:ILE:HD11 | 79:DT:190:ILE:HD12 | 1.74                     | 0.70              |
| 79:DT:118:LYS:HA   | 79:DT:118:LYS:HE3  | 1.73                     | 0.70              |
| 1:1:252:U:H5'      | 1:1:253:A:C8       | 2.26                     | 0.70              |
| 1:1:1841:G:H5''    | 1:1:1842:C:H5'     | 1.72                     | 0.70              |
| 46:B:1743:A:OP1    | 86:B:1851:GET:H311 | 1.91                     | 0.70              |
| 1:AS:833:A:OP2     | 44:CK:4:ARG:NH1    | 2.24                     | 0.70              |
| 8:BA:3:GLN:HG2     | 33:BZ:76:LEU:H     | 1.56                     | 0.70              |
| 66:DG:130:ARG:NH1  | 66:DG:131:ASP:OD1  | 2.24                     | 0.70              |
| 1:1:1229:G:N2      | 82:12:131:GLU:OE2  | 2.25                     | 0.70              |
| 1:1:1479:G:O6      | 35:AH:4:ARG:NH2    | 2.25                     | 0.70              |
| 27:9:51:ARG:HG2    | 27:9:52:GLN:H      | 1.57                     | 0.70              |
| 14:BG:67:ARG:HD2   | 29:BV:105:LEU:O    | 1.92                     | 0.70              |
| 64:DE:25:THR:HG23  | 64:DE:27:ASP:H     | 1.57                     | 0.70              |
| 82:12:103:ASN:C    | 82:12:105:PRO:HD3  | 2.17                     | 0.70              |
| 1:1:1058:A:O2'     | 22:2:108:ARG:NH2   | 2.24                     | 0.70              |
| 46:B:1354:U:N3     | 46:B:1355:A:N7     | 2.40                     | 0.70              |
| 65:U:16:ARG:NH1    | 65:U:21:ASN:OD1    | 2.25                     | 0.70              |
| 46:CM:1542:A:OP2   | 62:DC:47:ARG:NH2   | 2.15                     | 0.70              |
| 52:CS:146:SER:HB3  | 52:CS:221:ALA:HA   | 1.74                     | 0.70              |
| 59:CZ:63:CYS:SG    | 59:CZ:94:ALA:HB2   | 2.31                     | 0.70              |
| 1:AS:3136:C:H2'    | 1:AS:3137:A:C8     | 2.27                     | 0.69              |
| 7:AZ:197:LYS:HG2   | 7:AZ:202:GLY:HA3   | 1.73                     | 0.69              |
| 50:CQ:128:MET:HE1  | 50:CQ:134:GLY:HA2  | 1.73                     | 0.69              |
| 59:CZ:75:VAL:HA    | 59:CZ:78:LEU:HD23  | 1.73                     | 0.69              |
| 79:DT:113:SER:CB   | 79:DT:154:ALA:HA   | 2.22                     | 0.69              |
| 81:P0:60:ARG:O     | 81:P0:64:ARG:N     | 2.22                     | 0.69              |
| 46:B:1668:A:H8     | 53:I:65:GLN:HG3    | 1.57                     | 0.69              |
| 46:B:1741:A:C6     | 86:B:1851:GET:H21  | 2.27                     | 0.69              |
| 1:AS:763:U:H4'     | 14:BG:188:ARG:HH12 | 1.58                     | 0.69              |
| 25:BR:96:GLN:CG    | 25:BR:99:SER:HB2   | 2.20                     | 0.69              |
| 46:B:70:C:OP2      | 53:I:164:LYS:NZ    | 2.25                     | 0.69              |
| 49:E:165:ILE:HB    | 49:E:192:TYR:HB2   | 1.74                     | 0.69              |
| 68:DI:64:GLU:OE2   | 74:DO:2:VAL:N      | 2.25                     | 0.69              |
| 55:K:136:VAL:O     | 55:K:141:ARG:NH2   | 2.24                     | 0.69              |
| 1:AS:589:G:N2      | 1:AS:610:U:OP1     | 2.25                     | 0.69              |
| 1:AS:1134:U:O4     | 30:BW:10:HIS:NE2   | 2.25                     | 0.69              |
| 1:AS:1673:G:H5'    | 23:BP:100:SER:HB3  | 1.73                     | 0.69              |
| 48:CO:171:ILE:O    | 48:CO:175:GLU:HG2  | 1.91                     | 0.69              |
| 46:B:64:U:O2'      | 46:B:166:A:N3      | 2.24                     | 0.69              |
| 46:B:1487:C:P      | 66:V:122:ARG:HH22  | 2.15                     | 0.69              |
| 70:Z:107:PHE:CE2   | 70:Z:114:LYS:HD3   | 2.27                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:AR:90:LEU:HB2  | 79:AR:104:PHE:HB2 | 1.75                     | 0.69              |
| 1:AS:2191:A:H2'   | 1:AS:2192:A:H8    | 1.56                     | 0.69              |
| 1:1:627:U:H2'     | 1:1:628:A:C8      | 2.28                     | 0.69              |
| 1:1:1895:G:O2'    | 1:1:2312:U:O4     | 2.09                     | 0.69              |
| 4:j:101:ILE:HG12  | 4:j:165:VAL:HG22  | 1.74                     | 0.69              |
| 77:g:50:THR:OG1   | 77:g:53:LYS:HB2   | 1.91                     | 0.69              |
| 1:AS:1870:A:OP2   | 20:BM:20:ARG:NH1  | 2.25                     | 0.69              |
| 1:AS:2155:G:OP2   | 4:AW:128:ARG:NH1  | 2.25                     | 0.69              |
| 57:CX:54:TYR:HD1  | 57:CX:72:GLY:HA2  | 1.57                     | 0.69              |
| 59:CZ:102:GLY:C   | 59:CZ:104:CYS:H   | 2.01                     | 0.69              |
| 1:1:429:U:H2'     | 1:1:430:G:H8      | 1.55                     | 0.69              |
| 1:1:2915:G:OP2    | 5:k:2:SER:OG      | 2.09                     | 0.69              |
| 7:m:155:THR:HG22  | 7:m:179:ARG:HD3   | 1.73                     | 0.69              |
| 45:i:73:VAL:HG23  | 45:i:74:ALA:H     | 1.57                     | 0.69              |
| 45:i:96:LYS:HG3   | 46:B:575:G:C5     | 2.28                     | 0.69              |
| 48:D:77:GLU:OE2   | 61:Q:109:ARG:NH1  | 2.20                     | 0.69              |
| 73:c:7:SER:OG     | 73:c:10:ARG:O     | 2.11                     | 0.69              |
| 45:CL:65:LYS:NZ   | 62:DC:103:ASN:OD1 | 2.24                     | 0.69              |
| 46:CM:345:G:H5''  | 58:CY:85:ILE:HD11 | 1.75                     | 0.69              |
| 46:CM:1784:A:H5'  | 73:DN:95:ARG:HG2  | 1.73                     | 0.69              |
| 54:CU:13:LEU:HA   | 54:CU:16:LYS:HG2  | 1.74                     | 0.69              |
| 62:DC:86:VAL:H    | 62:DC:89:MET:HE2  | 1.58                     | 0.69              |
| 1:1:1662:G:H2'    | 1:1:1663:A:C8     | 2.27                     | 0.69              |
| 83:1:3401:3K5:H39 | 83:1:3401:3K5:H16 | 1.75                     | 0.69              |
| 4:j:27:ALA:O      | 4:j:128:ARG:NH2   | 2.25                     | 0.69              |
| 15:u:17:ARG:NH2   | 15:u:58:THR:O     | 2.25                     | 0.69              |
| 19:y:96:PHE:O     | 19:y:117:ASN:ND2  | 2.24                     | 0.69              |
| 50:F:223:THR:HG21 | 79:AR:225:ASN:HB3 | 1.74                     | 0.69              |
| 52:H:109:LYS:O    | 52:H:113:ILE:HD12 | 1.92                     | 0.69              |
| 54:J:5:ILE:HG21   | 54:J:10:PRO:HB3   | 1.75                     | 0.69              |
| 55:K:158:ILE:HD11 | 55:K:163:ASP:OD1  | 1.92                     | 0.69              |
| 59:O:36:LEU:HG    | 59:O:102:GLY:HA3  | 1.74                     | 0.69              |
| 1:AS:278:U:H3     | 1:AS:287:G:H1     | 1.41                     | 0.69              |
| 1:AS:1662:G:H2'   | 1:AS:1663:A:H8    | 1.58                     | 0.69              |
| 1:AS:1882:A:O2'   | 5:AX:226:PHE:O    | 2.11                     | 0.69              |
| 6:AY:36:VAL:HG21  | 6:AY:245:LEU:HD21 | 1.75                     | 0.69              |
| 7:AZ:91:GLY:O     | 7:AZ:94:ASN:ND2   | 2.26                     | 0.69              |
| 46:CM:122:U:H2'   | 46:CM:123:G:H5''  | 1.74                     | 0.69              |
| 46:CM:211:A:H62   | 46:CM:250:U:H3    | 1.40                     | 0.69              |
| 46:CM:317:U:H4'   | 46:CM:321:A:C8    | 2.28                     | 0.69              |
| 46:CM:369:G:N1    | 46:CM:611:G:O6    | 2.19                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:509:A:OP2    | 56:CW:176:ASN:ND2  | 2.26                     | 0.69              |
| 46:CM:741:A:H5'    | 51:CR:16:SER:HB3   | 1.75                     | 0.69              |
| 46:CM:826:U:H2'    | 46:CM:827:C:H5'    | 1.75                     | 0.69              |
| 46:CM:872:A:H1'    | 61:DB:117:PRO:HB3  | 1.75                     | 0.69              |
| 46:CM:1334:G:N3    | 46:CM:1365:C:N4    | 2.41                     | 0.69              |
| 79:DT:209:ALA:H    | 79:DT:242:PHE:HE1  | 1.39                     | 0.69              |
| 1:1:617:A:H5'      | 1:1:619:A:H1'      | 1.75                     | 0.69              |
| 1:1:2171:U:H5'     | 1:1:2172:G:H5'     | 1.75                     | 0.69              |
| 46:B:78:A:H2       | 53:I:174:LYS:HG3   | 1.57                     | 0.69              |
| 46:B:728:U:OP1     | 54:J:104:LYS:N     | 2.26                     | 0.69              |
| 52:H:200:ASN:HB3   | 52:H:208:SER:HB3   | 1.74                     | 0.69              |
| 60:P:54:LEU:HB3    | 60:P:60:VAL:HB     | 1.75                     | 0.69              |
| 46:CM:1152:G:N2    | 63:DD:138:GLN:HE22 | 1.91                     | 0.69              |
| 3:4:103:G:OP2      | 3:4:105:A:O2'      | 2.11                     | 0.69              |
| 46:B:345:G:H5''    | 58:N:85:ILE:HD11   | 1.74                     | 0.69              |
| 46:B:1350:C:H5''   | 63:S:27:LEU:HD22   | 1.75                     | 0.69              |
| 56:L:106:GLU:O     | 56:L:112:GLN:NE2   | 2.24                     | 0.69              |
| 1:AS:595:G:OP2     | 9:BB:32:LYS:NZ     | 2.26                     | 0.69              |
| 46:CM:1485:G:N1    | 46:CM:1496:C:N3    | 2.34                     | 0.69              |
| 63:DD:12:LYS:HG3   | 63:DD:13:LYS:H     | 1.58                     | 0.69              |
| 1:1:1473:A:OP1     | 1:1:3047:G:O2'     | 2.08                     | 0.68              |
| 46:B:1335:U:H2'    | 46:B:1336:G:C8     | 2.28                     | 0.68              |
| 63:S:34:PRO:HB2    | 63:S:36:THR:HG22   | 1.75                     | 0.68              |
| 1:AS:297:G:OP2     | 1:AS:297:G:N2      | 2.21                     | 0.68              |
| 48:CO:70:LEU:HD23  | 48:CO:79:HIS:HD2   | 1.58                     | 0.68              |
| 54:CU:6:LEU:HB2    | 54:CU:40:LYS:HA    | 1.75                     | 0.68              |
| 1:AS:2932:C:H2'    | 1:AS:2933:G:H8     | 1.58                     | 0.68              |
| 1:AS:3195:G:H4'    | 15:BH:125:LYS:HE2  | 1.75                     | 0.68              |
| 1:AS:3245:A:HO2'   | 1:AS:3246:C:H6     | 1.41                     | 0.68              |
| 46:CM:834:C:H2'    | 46:CM:835:A:C8     | 2.28                     | 0.68              |
| 46:CM:1026:G:H2'   | 46:CM:1027:G:C8    | 2.28                     | 0.68              |
| 55:CV:120:THR:HG21 | 55:CV:133:ALA:HA   | 1.73                     | 0.68              |
| 65:DF:134:ARG:HB2  | 65:DF:136:GLN:HE22 | 1.58                     | 0.68              |
| 79:DT:150:ASP:H    | 79:DT:172:ASP:HB3  | 1.58                     | 0.68              |
| 1:1:307:A:H2'      | 1:1:308:A:C8       | 2.28                     | 0.68              |
| 1:1:1231:U:H4'     | 1:1:1232:G:H5'     | 1.74                     | 0.68              |
| 46:B:578:A:O2'     | 46:B:580:U:OP1     | 2.11                     | 0.68              |
| 59:O:40:GLY:HA2    | 59:O:124:LYS:CG    | 2.22                     | 0.68              |
| 80:BE:43:VAL:HG21  | 80:BE:197:VAL:HG13 | 1.76                     | 0.68              |
| 62:DC:17:PHE:O     | 62:DC:19:GLY:N     | 2.26                     | 0.68              |
| 57:M:80:LEU:HB3    | 57:M:82:ILE:HG23   | 1.76                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:f:39:CYS:HB3    | 76:f:41:GLN:H      | 1.59                     | 0.68              |
| 10:BC:113:GLU:O    | 10:BC:117:ILE:HG13 | 1.93                     | 0.68              |
| 25:BR:102:LYS:CE   | 25:BR:105:ARG:NH2  | 2.52                     | 0.68              |
| 1:1:1804:G:OP2     | 28:AA:133:LYS:NZ   | 2.26                     | 0.68              |
| 3:4:38:U:O2'       | 36:AI:83:LYS:NZ    | 2.24                     | 0.68              |
| 49:E:53:LEU:HA     | 68:X:12:TYR:HE1    | 1.57                     | 0.68              |
| 15:BH:17:ARG:NH2   | 15:BH:58:THR:O     | 2.27                     | 0.68              |
| 39:CF:31:VAL:HA    | 39:CF:38:PHE:HB3   | 1.74                     | 0.68              |
| 46:CM:1592:G:OP2   | 63:DD:126:LYS:NZ   | 2.24                     | 0.68              |
| 82:12:104:ILE:N    | 82:12:105:PRO:HD3  | 2.09                     | 0.68              |
| 6:l:303:ALA:HB2    | 19:y:39:ARG:HH12   | 1.58                     | 0.68              |
| 46:B:1144:C:N4     | 46:B:1270:U:OP1    | 2.27                     | 0.68              |
| 62:R:81:ARG:NH2    | 62:R:117:GLY:O     | 2.27                     | 0.68              |
| 3:AU:154:C:H5''    | 10:BC:182:LYS:HD3  | 1.74                     | 0.68              |
| 32:BY:71:ARG:HH11  | 32:BY:103:LEU:HD13 | 1.59                     | 0.68              |
| 62:DC:28:MET:HE1   | 62:DC:36:LEU:HD21  | 1.74                     | 0.68              |
| 46:B:671:G:H5''    | 46:B:672:U:C6      | 2.29                     | 0.68              |
| 47:C:147:THR:HG21  | 47:C:159:ALA:HB1   | 1.75                     | 0.68              |
| 79:AR:52:ASP:O     | 79:AR:53:ASN:ND2   | 2.27                     | 0.68              |
| 1:AS:654:A:H2'     | 1:AS:655:A:C8      | 2.29                     | 0.68              |
| 33:BZ:97:ILE:HG21  | 33:BZ:106:ARG:HG3  | 1.75                     | 0.68              |
| 64:DE:37:GLU:OE1   | 79:DT:151:TRP:NE1  | 2.27                     | 0.68              |
| 5:k:35:ASP:OD2     | 5:k:191:LYS:NZ     | 2.17                     | 0.68              |
| 1:AS:365:A:OP1     | 6:AY:85:ARG:NH1    | 2.27                     | 0.68              |
| 1:AS:2645:A:O2'    | 13:BF:126:ASP:OD1  | 2.09                     | 0.68              |
| 19:BL:96:PHE:O     | 19:BL:117:ASN:ND2  | 2.27                     | 0.68              |
| 22:BO:108:ARG:O    | 22:BO:112:ASN:ND2  | 2.27                     | 0.68              |
| 35:CB:57:LEU:HB2   | 35:CB:62:TYR:CE1   | 2.29                     | 0.68              |
| 46:CM:255:A:N3     | 55:CV:64:ASN:ND2   | 2.40                     | 0.68              |
| 46:CM:855:C:O2     | 74:DO:51:GLN:NE2   | 2.27                     | 0.68              |
| 46:CM:1600:U:OP1   | 52:CS:169:ASN:HB2  | 1.93                     | 0.68              |
| 46:CM:1741:A:H1'   | 77:DR:3:LYS:HG3    | 1.74                     | 0.68              |
| 48:CO:225:LEU:O    | 48:CO:229:LEU:HG   | 1.93                     | 0.68              |
| 52:CS:205:SER:O    | 52:CS:207:THR:N    | 2.27                     | 0.68              |
| 79:DT:145:LEU:HD21 | 79:DT:178:TRP:CE2  | 2.29                     | 0.68              |
| 79:DT:198:CYS:CB   | 79:DT:239:ALA:HA   | 2.24                     | 0.68              |
| 1:1:581:A:H5''     | 34:AG:106:ASN:ND2  | 2.08                     | 0.68              |
| 46:CM:850:A:OP1    | 69:DJ:28:ARG:NH2   | 2.27                     | 0.68              |
| 62:DC:29:PRO:HG2   | 62:DC:32:GLU:HB2   | 1.74                     | 0.68              |
| 64:T:27:ASP:O      | 64:T:31:ASN:ND2    | 2.27                     | 0.68              |
| 79:AR:50:GLY:H     | 79:AR:55:TYR:HA    | 1.59                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:CU:94:ILE:HG12  | 54:CU:117:VAL:HG21 | 1.74                     | 0.68              |
| 1:1:2650:A:C2      | 45:i:52:LYS:HA     | 2.29                     | 0.67              |
| 1:AS:1774:G:O2'    | 1:AS:1776:G:OP2    | 2.11                     | 0.67              |
| 4:AW:51:ASP:OD2    | 4:AW:54:ARG:NH2    | 2.27                     | 0.67              |
| 46:CM:1282:G:N2    | 46:CM:1285:A:OP2   | 2.19                     | 0.67              |
| 46:CM:1669:U:O4    | 46:CM:1707:G:N2    | 2.27                     | 0.67              |
| 81:P0:37:GLN:NE2   | 81:P0:103:ASN:O    | 2.27                     | 0.67              |
| 1:1:647:A:OP2      | 1:1:2840:U:O2'     | 2.11                     | 0.67              |
| 5:k:372:THR:HG22   | 5:k:374:ALA:H      | 1.58                     | 0.67              |
| 1:AS:447:U:C2'     | 1:AS:448:U:H5''    | 2.21                     | 0.67              |
| 46:CM:880:G:O2'    | 61:DB:33:THR:N     | 2.19                     | 0.67              |
| 46:CM:1324:C:O2'   | 46:CM:1326:A:N7    | 2.26                     | 0.67              |
| 69:DJ:7:LEU:HD11   | 69:DJ:37:PHE:HD2   | 1.59                     | 0.67              |
| 82:12:162:VAL:HG12 | 82:12:164:GLU:CG   | 2.24                     | 0.67              |
| 1:1:1713:U:H2'     | 1:1:1714:G:C8      | 2.29                     | 0.67              |
| 46:B:589:A:H2'     | 46:B:590:A:C8      | 2.29                     | 0.67              |
| 64:T:103:ASP:OD1   | 64:T:104:ALA:N     | 2.27                     | 0.67              |
| 73:c:5:ARG:HD3     | 73:c:9:GLY:N       | 2.09                     | 0.67              |
| 1:AS:653:C:H2'     | 1:AS:654:A:C8      | 2.28                     | 0.67              |
| 16:BI:159:ARG:HB2  | 16:BI:164:LEU:HB2  | 1.75                     | 0.67              |
| 27:BT:44:ASN:HB2   | 27:BT:125:LYS:NZ   | 2.09                     | 0.67              |
| 50:CQ:212:ALA:HB2  | 64:DE:19:ARG:HG3   | 1.76                     | 0.67              |
| 59:CZ:89:ILE:HD13  | 59:CZ:140:PHE:CD1  | 2.29                     | 0.67              |
| 78:DS:124:LYS:NZ   | 78:DS:126:VAL:H    | 1.91                     | 0.67              |
| 79:DT:16:HIS:CE1   | 79:DT:37:SER:HB2   | 2.29                     | 0.67              |
| 79:DT:198:CYS:HB3  | 79:DT:239:ALA:HA   | 1.76                     | 0.67              |
| 79:DT:262:LEU:CD2  | 79:DT:263:GLN:H    | 2.07                     | 0.67              |
| 1:1:358:G:N2       | 1:1:361:A:OP2      | 2.25                     | 0.67              |
| 1:1:2812:C:N4      | 1:1:2817:A:O2'     | 2.27                     | 0.67              |
| 1:AS:447:U:O2'     | 1:AS:448:U:OP1     | 2.12                     | 0.67              |
| 46:CM:1276:G:H1    | 46:CM:1309:G:H22   | 1.40                     | 0.67              |
| 46:CM:1579:A:H2'   | 46:CM:1580:A:H8    | 1.58                     | 0.67              |
| 48:CO:48:ILE:HD12  | 48:CO:61:LEU:HD13  | 1.76                     | 0.67              |
| 59:CZ:97:LEU:HD13  | 59:CZ:119:SER:HA   | 1.76                     | 0.67              |
| 82:12:128:VAL:O    | 82:12:132:ILE:HG13 | 1.94                     | 0.67              |
| 1:1:654:A:H2'      | 1:1:655:A:H8       | 1.59                     | 0.67              |
| 1:1:1344:U:OP1     | 19:y:39:ARG:NH2    | 2.28                     | 0.67              |
| 1:1:2516:U:O2'     | 1:1:2519:A:N1      | 2.27                     | 0.67              |
| 46:B:635:C:O2      | 54:J:110:ARG:NH2   | 2.24                     | 0.67              |
| 46:B:903:U:H2'     | 46:B:904:A:C8      | 2.29                     | 0.67              |
| 1:AS:925:A:O2'     | 38:CE:49:TRP:O     | 2.13                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AU:13:A:O2'      | 18:BK:121:HIS:O    | 2.11                     | 0.67              |
| 10:BC:141:VAL:HG22 | 10:BC:167:LEU:HD21 | 1.77                     | 0.67              |
| 14:BG:48:PRO:O     | 14:BG:49:ARG:C     | 2.36                     | 0.67              |
| 15:BH:14:GLU:HG2   | 15:BH:17:ARG:HG2   | 1.75                     | 0.67              |
| 39:CF:71:PRO:O     | 39:CF:73:LEU:N     | 2.28                     | 0.67              |
| 48:CO:90:GLU:HG2   | 48:CO:97:LEU:HG    | 1.76                     | 0.67              |
| 69:DJ:2:THR:HG22   | 69:DJ:3:ARG:N      | 2.09                     | 0.67              |
| 78:DS:174:MET:SD   | 78:DS:183:CYS:HB2  | 2.33                     | 0.67              |
| 78:DS:174:MET:HE3  | 78:DS:190:LEU:HD23 | 1.77                     | 0.67              |
| 79:DT:261:LYS:HB2  | 79:DT:266:SER:HB2  | 1.75                     | 0.67              |
| 1:l:383:G:N2       | 1:l:386:A:OP2      | 2.28                     | 0.67              |
| 36:AI:64:GLU:HA    | 36:AI:67:ARG:HB2   | 1.76                     | 0.67              |
| 46:B:1156:A:H2'    | 46:B:1157:G:H8     | 1.57                     | 0.67              |
| 71:a:10:ARG:NH1    | 71:a:26:ASP:OD2    | 2.26                     | 0.67              |
| 14:BG:195:ALA:O    | 14:BG:199:LYS:HB2  | 1.95                     | 0.67              |
| 23:BP:59:GLU:CD    | 23:BP:60:SER:H     | 2.02                     | 0.67              |
| 1:AS:2932:C:H2'    | 1:AS:2933:G:C8     | 2.30                     | 0.67              |
| 39:CF:8:ILE:HD13   | 39:CF:54:LEU:HD21  | 1.77                     | 0.67              |
| 49:CP:96:VAL:HG22  | 49:CP:110:ILE:HG12 | 1.76                     | 0.67              |
| 50:CQ:49:VAL:HB    | 50:CQ:87:ILE:HD13  | 1.75                     | 0.67              |
| 79:DT:74:ILE:HG22  | 79:DT:75:SER:H     | 1.59                     | 0.67              |
| 14:t:48:PRO:HD3    | 14:t:135:VAL:HG13  | 1.77                     | 0.67              |
| 66:V:127:ASN:HB3   | 66:V:130:ARG:HH21  | 1.59                     | 0.67              |
| 1:AS:1344:U:OP1    | 19:BL:39:ARG:NH2   | 2.27                     | 0.67              |
| 1:AS:1631:G:N2     | 1:AS:1634:A:OP2    | 2.23                     | 0.67              |
| 10:BC:212:LEU:O    | 10:BC:216:ILE:HG12 | 1.95                     | 0.67              |
| 45:CL:52:LYS:HA    | 45:CL:52:LYS:HE3   | 1.77                     | 0.67              |
| 46:CM:1067:C:H4'   | 68:DI:58:TYR:CE1   | 2.26                     | 0.67              |
| 48:CO:24:PHE:HA    | 48:CO:27:LYS:HG2   | 1.77                     | 0.67              |
| 48:CO:144:LYS:HG3  | 48:CO:208:GLN:HB3  | 1.76                     | 0.67              |
| 16:v:23:TYR:O      | 16:v:122:ASN:ND2   | 2.26                     | 0.67              |
| 46:B:1216:U:H3     | 46:B:1239:U:H3     | 1.43                     | 0.67              |
| 63:S:98:GLU:HG3    | 63:S:101:LYS:HE3   | 1.77                     | 0.67              |
| 1:AS:1936:G:H21    | 1:AS:3327:A:H8     | 1.42                     | 0.67              |
| 1:AS:2233:A:HO2'   | 46:CM:1744:G:HO2'  | 1.36                     | 0.67              |
| 23:BP:50:LEU:HG    | 23:BP:54:ILE:HD12  | 1.75                     | 0.67              |
| 28:BU:90:GLU:HA    | 28:BU:93:LYS:HD3   | 1.75                     | 0.67              |
| 45:CL:100:LYS:H    | 45:CL:100:LYS:HD2  | 1.60                     | 0.67              |
| 54:CU:160:TYR:HE2  | 54:CU:161:LYS:NZ   | 1.92                     | 0.67              |
| 6:l:6:GLN:HB3      | 6:l:20:GLN:HB3     | 1.76                     | 0.67              |
| 1:AS:3162:U:N3     | 1:AS:3166:A:H2     | 1.93                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BP:101:VAL:HG11 | 23:BP:107:LYS:NZ   | 2.10                     | 0.67              |
| 46:CM:217:A:N7     | 46:CM:816:U:C2     | 2.63                     | 0.67              |
| 46:CM:482:C:H2'    | 46:CM:483:A:C8     | 2.29                     | 0.67              |
| 46:CM:786:G:H21    | 69:DJ:107:SER:HB3  | 1.60                     | 0.67              |
| 46:CM:812:C:H2'    | 46:CM:813:U:C6     | 2.30                     | 0.67              |
| 46:CM:876:A:H2'    | 46:CM:877:G:H8     | 1.60                     | 0.67              |
| 46:CM:1339:G:O6    | 46:CM:1354:U:O2    | 2.12                     | 0.67              |
| 54:CU:3:SER:O      | 54:CU:38:GLN:NE2   | 2.28                     | 0.67              |
| 62:DC:41:VAL:HG12  | 62:DC:45:PHE:HE2   | 1.59                     | 0.67              |
| 82:12:114:ARG:HH21 | 82:12:125:LEU:HD13 | 1.60                     | 0.67              |
| 1:1:1591:U:O2'     | 1:1:1602:U:O2      | 2.12                     | 0.66              |
| 1:1:2694:U:O2'     | 22:2:88:ARG:O      | 2.10                     | 0.66              |
| 1:1:3199:G:N2      | 1:1:3218:U:O2      | 2.24                     | 0.66              |
| 1:1:3235:A:O4'     | 18:x:174:GLY:HA3   | 1.95                     | 0.66              |
| 20:z:170:ARG:O     | 20:z:174:GLN:HG2   | 1.96                     | 0.66              |
| 48:D:190:PRO:HG2   | 48:D:192:VAL:HG23  | 1.75                     | 0.66              |
| 68:X:38:LYS:HD2    | 68:X:49:GLU:HG3    | 1.76                     | 0.66              |
| 1:AS:843:A:H2'     | 1:AS:844:A:C8      | 2.31                     | 0.66              |
| 46:CM:57:G:OP1     | 71:DL:112:LYS:NZ   | 2.28                     | 0.66              |
| 46:CM:327:G:H5''   | 55:CV:98:LYS:HB3   | 1.76                     | 0.66              |
| 47:CN:59:LEU:HD22  | 68:DI:79:LEU:HD11  | 1.76                     | 0.66              |
| 48:CO:100:PHE:HD2  | 48:CO:181:LEU:HD11 | 1.58                     | 0.66              |
| 59:CZ:69:GLU:HB2   | 59:CZ:72:ILE:HD12  | 1.77                     | 0.66              |
| 62:DC:63:ALA:HB1   | 62:DC:73:PRO:O     | 1.95                     | 0.66              |
| 1:1:438:A:N1       | 1:1:489:G:O2'      | 2.24                     | 0.66              |
| 1:AS:2194:G:N2     | 1:AS:2207:A:N1     | 2.42                     | 0.66              |
| 42:CI:11:ARG:NH2   | 46:CM:1762:U:OP1   | 2.29                     | 0.66              |
| 46:CM:217:A:H61    | 46:CM:828:U:H1'    | 1.59                     | 0.66              |
| 48:CO:70:LEU:HD23  | 48:CO:79:HIS:CD2   | 2.30                     | 0.66              |
| 54:CU:47:VAL:HG23  | 54:CU:48:ASN:H     | 1.60                     | 0.66              |
| 69:DJ:75:ILE:HD11  | 69:DJ:93:LEU:HD11  | 1.78                     | 0.66              |
| 79:DT:12:THR:O     | 79:DT:53:ASN:HA    | 1.95                     | 0.66              |
| 1:1:378:A:N6       | 1:1:391:A:O2'      | 2.29                     | 0.66              |
| 30:AC:58:ARG:HG2   | 30:AC:59:ALA:H     | 1.60                     | 0.66              |
| 46:B:853:G:OP1     | 60:P:121:ARG:NH1   | 2.28                     | 0.66              |
| 1:AS:2717:G:N2     | 1:AS:2720:A:OP2    | 2.25                     | 0.66              |
| 23:BP:19:VAL:O     | 23:BP:22:PRO:HD2   | 1.96                     | 0.66              |
| 28:BU:94:SER:O     | 28:BU:97:THR:HG23  | 1.95                     | 0.66              |
| 37:CD:59:LEU:HG    | 37:CD:68:ALA:CB    | 2.26                     | 0.66              |
| 45:CL:105:GLN:OE1  | 45:CL:113:ARG:NH1  | 2.25                     | 0.66              |
| 46:CM:824:U:N3     | 46:CM:825:U:O4     | 2.28                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1235:U:O2'   | 78:DS:177:MET:HB2  | 1.95                     | 0.66              |
| 1:1:171:G:N2       | 1:1:246:U:O2       | 2.27                     | 0.66              |
| 1:1:531:G:HO2'     | 1:1:552:G:H1       | 1.43                     | 0.66              |
| 46:CM:1216:U:H3    | 46:CM:1239:U:H3    | 1.42                     | 0.66              |
| 55:CV:201:ARG:HH12 | 58:CY:11:ARG:HA    | 1.60                     | 0.66              |
| 67:DH:52:LYS:HB3   | 67:DH:91:ASP:HB2   | 1.76                     | 0.66              |
| 46:B:847:A:O2'     | 46:B:948:A:N1      | 2.27                     | 0.66              |
| 1:AS:292:U:OP2     | 16:BI:68:ARG:NH2   | 2.26                     | 0.66              |
| 13:BF:109:HIS:HD2  | 13:BF:123:TYR:H    | 1.43                     | 0.66              |
| 20:BM:176:ARG:NH1  | 20:BM:180:LYS:HB2  | 2.02                     | 0.66              |
| 50:CQ:107:LYS:HB2  | 50:CQ:176:VAL:HG22 | 1.76                     | 0.66              |
| 59:CZ:81:GLU:OE1   | 78:DS:155:ASN:ND2  | 2.29                     | 0.66              |
| 63:DD:28:ILE:HG22  | 63:DD:64:ILE:HB    | 1.77                     | 0.66              |
| 46:B:784:U:H2'     | 46:B:785:G:H8      | 1.60                     | 0.66              |
| 54:J:146:GLN:HB2   | 54:J:177:VAL:HG23  | 1.76                     | 0.66              |
| 63:S:26:GLY:HA2    | 63:S:62:ILE:O      | 1.95                     | 0.66              |
| 1:AS:763:U:H4'     | 14:BG:188:ARG:NH1  | 2.10                     | 0.66              |
| 1:AS:2254:G:OP1    | 42:CI:16:LYS:NZ    | 2.28                     | 0.66              |
| 1:AS:2520:A:H1'    | 1:AS:2521:C:H5     | 1.60                     | 0.66              |
| 1:AS:2752:A:OP1    | 14:BG:179:LYS:NZ   | 2.29                     | 0.66              |
| 7:AZ:85:ARG:NH2    | 7:AZ:250:ASP:OD2   | 2.27                     | 0.66              |
| 8:BA:39:LEU:HB3    | 8:BA:83:VAL:HG13   | 1.78                     | 0.66              |
| 23:BP:37:LEU:HD11  | 23:BP:56:ILE:HD13  | 1.78                     | 0.66              |
| 52:CS:133:VAL:O    | 52:CS:137:ILE:HG13 | 1.94                     | 0.66              |
| 1:1:2869:A:OP2     | 41:AN:48:LYS:NZ    | 2.29                     | 0.66              |
| 25:7:108:LYS:NZ    | 53:I:154:ARG:HD3   | 2.11                     | 0.66              |
| 46:B:605:G:H5'     | 46:B:611:G:N2      | 2.10                     | 0.66              |
| 46:B:1422:A:OP2    | 50:F:28:ARG:NH2    | 2.29                     | 0.66              |
| 25:BR:104:ALA:O    | 25:BR:108:LYS:HB3  | 1.96                     | 0.66              |
| 11:q:80:THR:HA     | 11:q:83:THR:HG22   | 1.77                     | 0.66              |
| 46:B:829:A:H2'     | 46:B:830:G:H8      | 1.59                     | 0.66              |
| 47:C:41:ARG:HD3    | 47:C:47:ILE:HD11   | 1.76                     | 0.66              |
| 1:AS:2370:C:H1'    | 5:AX:266:ARG:HH21  | 1.60                     | 0.66              |
| 1:AS:3156:A:O2'    | 11:BD:23:ARG:NH1   | 2.29                     | 0.66              |
| 10:BC:139:HIS:CE1  | 10:BC:143:LEU:HD11 | 2.30                     | 0.66              |
| 28:BU:53:VAL:HG11  | 28:BU:62:VAL:HG13  | 1.76                     | 0.66              |
| 46:CM:148:C:H42    | 46:CM:162:A:H61    | 1.41                     | 0.66              |
| 46:CM:880:G:H1     | 46:CM:902:U:H3     | 1.44                     | 0.66              |
| 46:CM:1341:U:H1'   | 46:CM:1353:G:N2    | 2.11                     | 0.66              |
| 1:1:3133:G:H2'     | 1:1:3134:C:H6      | 1.61                     | 0.66              |
| 6:l:266:ASP:O      | 6:l:267:SER:HB3    | 1.95                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:960:C:H5''   | 60:P:109:LYS:HD3   | 1.78                     | 0.66              |
| 1:AS:431:A:H2'    | 1:AS:432:G:C8      | 2.31                     | 0.66              |
| 46:CM:1156:A:H2'  | 46:CM:1157:G:H8    | 1.57                     | 0.66              |
| 48:CO:220:GLN:CD  | 48:CO:221:PRO:HD2  | 2.20                     | 0.66              |
| 1:1:2867:G:O2'    | 41:AN:24:TYR:O     | 2.13                     | 0.66              |
| 12:r:30:LYS:HG3   | 12:r:63:GLU:HG3    | 1.76                     | 0.66              |
| 57:M:86:ILE:HG13  | 57:M:87:LEU:HG     | 1.77                     | 0.66              |
| 1:AS:2812:C:N4    | 1:AS:2817:A:O2'    | 2.29                     | 0.66              |
| 46:CM:589:A:H2'   | 46:CM:590:A:C8     | 2.31                     | 0.66              |
| 55:CV:139:ALA:HB3 | 55:CV:141:ARG:HH12 | 1.60                     | 0.66              |
| 79:DT:46:LYS:HG3  | 79:DT:59:LYS:HE3   | 1.78                     | 0.66              |
| 79:DT:132:VAL:HB  | 79:DT:145:LEU:HD22 | 1.78                     | 0.66              |
| 1:1:279:U:O4      | 43:AP:45:ARG:NH2   | 2.29                     | 0.65              |
| 1:1:482:U:H2'     | 1:1:483:U:C6       | 2.31                     | 0.65              |
| 1:1:3287:A:H2'    | 1:1:3288:A:H8      | 1.61                     | 0.65              |
| 49:E:96:VAL:HG22  | 49:E:110:ILE:HG12  | 1.79                     | 0.65              |
| 1:AS:706:G:N2     | 1:AS:709:A:OP2     | 2.25                     | 0.65              |
| 23:BP:22:PRO:HB2  | 23:BP:28:PHE:HB2   | 1.78                     | 0.65              |
| 69:DJ:37:PHE:CE1  | 69:DJ:103:ILE:HG13 | 2.30                     | 0.65              |
| 16:v:31:ARG:NH1   | 16:v:124:ASP:OD2   | 2.28                     | 0.65              |
| 54:J:33:GLU:HG3   | 54:J:69:VAL:HG11   | 1.78                     | 0.65              |
| 1:AS:358:G:N2     | 1:AS:361:A:OP2     | 2.29                     | 0.65              |
| 1:AS:2603:U:OP2   | 22:BO:4:SER:OG     | 2.13                     | 0.65              |
| 1:AS:3287:A:H2'   | 1:AS:3288:A:C8     | 2.31                     | 0.65              |
| 28:BU:128:LYS:O   | 28:BU:132:GLN:HG2  | 1.95                     | 0.65              |
| 46:CM:218:A:H3'   | 46:CM:219:A:C5'    | 2.26                     | 0.65              |
| 46:CM:881:U:H5'   | 48:CO:23:PRO:HG2   | 1.79                     | 0.65              |
| 46:CM:1701:A:H2'  | 46:CM:1702:A:C8    | 2.32                     | 0.65              |
| 52:CS:203:LYS:HE2 | 52:CS:205:SER:HB2  | 1.78                     | 0.65              |
| 59:CZ:51:ALA:CB   | 59:CZ:122:VAL:HG11 | 2.27                     | 0.65              |
| 68:DI:58:TYR:OH   | 69:DJ:20:THR:HA    | 1.96                     | 0.65              |
| 1:1:1663:A:H2'    | 1:1:1664:G:C8      | 2.31                     | 0.65              |
| 1:1:1782:G:H2'    | 1:1:1783:A:C8      | 2.32                     | 0.65              |
| 28:AA:27:LYS:HE3  | 28:AA:97:THR:HG22  | 1.78                     | 0.65              |
| 46:B:115:G:H5'    | 58:N:129:ARG:HD3   | 1.78                     | 0.65              |
| 23:BP:50:LEU:HA   | 23:BP:54:ILE:HD11  | 1.78                     | 0.65              |
| 37:CD:50:ALA:N    | 37:CD:53:GLU:OE1   | 2.29                     | 0.65              |
| 46:CM:515:U:H2'   | 46:CM:516:A:H8     | 1.62                     | 0.65              |
| 48:CO:87:ARG:HH22 | 48:CO:133:TYR:HE2  | 1.42                     | 0.65              |
| 78:DS:124:LYS:HZ3 | 78:DS:126:VAL:H    | 1.44                     | 0.65              |
| 1:1:3254:G:H2'    | 1:1:3255:G:H8      | 1.61                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:p:101:GLU:HG2   | 10:p:105:GLU:HB3   | 1.79                     | 0.65              |
| 25:7:128:ALA:O     | 25:7:131:VAL:HG12  | 1.97                     | 0.65              |
| 27:9:40:ARG:HG3    | 27:9:45:VAL:O      | 1.95                     | 0.65              |
| 38:AK:28:HIS:HB3   | 38:AK:31:LYS:HB2   | 1.78                     | 0.65              |
| 46:B:1131:G:H2'    | 46:B:1132:A:C8     | 2.31                     | 0.65              |
| 53:I:163:THR:HA    | 53:I:168:THR:HG22  | 1.77                     | 0.65              |
| 56:L:31:ALA:HB2    | 56:L:42:ILE:HD11   | 1.77                     | 0.65              |
| 1:AS:1014:G:H1     | 1:AS:1030:U:H3     | 0.72                     | 0.65              |
| 1:AS:3179:U:H6     | 8:BA:166:LYS:HE2   | 1.60                     | 0.65              |
| 16:BI:42:PRO:HD3   | 16:BI:61:ILE:HG13  | 1.78                     | 0.65              |
| 46:CM:856:G:H2'    | 46:CM:857:G:C8     | 2.31                     | 0.65              |
| 47:CN:35:PRO:O     | 47:CN:52:LYS:NZ    | 2.28                     | 0.65              |
| 79:DT:208:CYS:HB3  | 79:DT:222:LEU:HD21 | 1.76                     | 0.65              |
| 68:X:70:ASN:HB3    | 68:X:83:TRP:HB2    | 1.79                     | 0.65              |
| 1:AS:412:G:H21     | 18:BK:118:GLN:HE22 | 1.43                     | 0.65              |
| 1:AS:2171:U:H5'    | 1:AS:2172:G:H5'    | 1.78                     | 0.65              |
| 1:AS:3135:A:H2'    | 1:AS:3136:C:C6     | 2.31                     | 0.65              |
| 2:AT:11:A:N6       | 7:AZ:16:PHE:O      | 2.29                     | 0.65              |
| 14:BG:32:LYS:HG2   | 14:BG:35:ARG:HH22  | 1.62                     | 0.65              |
| 50:CQ:222:PRO:HG2  | 79:DT:190:ILE:HD11 | 1.78                     | 0.65              |
| 62:DC:50:ASP:OD2   | 62:DC:52:LYS:HB2   | 1.97                     | 0.65              |
| 1:1:1936:G:H21     | 1:1:3327:A:H8      | 1.43                     | 0.65              |
| 46:B:759:A:H61     | 46:B:770:C:N4      | 1.95                     | 0.65              |
| 46:B:1578:C:H2'    | 46:B:1579:A:H8     | 1.61                     | 0.65              |
| 59:O:107:ASP:HB3   | 59:O:113:ARG:HG3   | 1.77                     | 0.65              |
| 1:AS:269:G:OP2     | 16:BI:44:ARG:NH1   | 2.30                     | 0.65              |
| 80:BE:54:SER:HB2   | 80:BE:135:ILE:HD11 | 1.78                     | 0.65              |
| 46:CM:972:G:N2     | 46:CM:998:A:OP1    | 2.27                     | 0.65              |
| 59:CZ:89:ILE:HD11  | 59:CZ:139:HIS:CE1  | 2.32                     | 0.65              |
| 1:1:591:C:O2       | 9:o:24:ARG:NH1     | 2.29                     | 0.65              |
| 1:1:834:G:O6       | 44:AQ:4:ARG:NH2    | 2.29                     | 0.65              |
| 46:B:1715:U:H2'    | 46:B:1716:C:C6     | 2.31                     | 0.65              |
| 51:G:129:VAL:HG22  | 51:G:139:VAL:HG22  | 1.79                     | 0.65              |
| 1:AS:827:G:O2'     | 1:AS:1860:A:N3     | 2.23                     | 0.65              |
| 46:CM:778:U:O2'    | 46:CM:779:U:O2     | 2.12                     | 0.65              |
| 46:CM:834:C:H2'    | 46:CM:835:A:H8     | 1.62                     | 0.65              |
| 48:CO:143:THR:HG22 | 48:CO:205:PHE:CE2  | 2.32                     | 0.65              |
| 62:DC:15:PHE:CB    | 62:DC:22:LEU:HB2   | 2.26                     | 0.65              |
| 1:1:1493:C:O2'     | 1:1:1598:A:N3      | 2.29                     | 0.65              |
| 14:t:115:ARG:NH2   | 14:t:147:PHE:O     | 2.29                     | 0.65              |
| 20:z:148:GLU:HG2   | 20:z:151:ARG:HH21  | 1.62                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:C:84:ARG:NH1   | 47:C:203:PHE:O    | 2.28                     | 0.65              |
| 1:AS:281:G:N7     | 16:BI:182:LYS:NZ  | 2.44                     | 0.65              |
| 1:AS:654:A:H2'    | 1:AS:655:A:H8     | 1.62                     | 0.65              |
| 1:AS:968:A:OP1    | 19:BL:12:ARG:NH2  | 2.30                     | 0.65              |
| 1:AS:2869:A:OP2   | 41:CH:48:LYS:NZ   | 2.29                     | 0.65              |
| 79:DT:197:SER:OG  | 79:DT:198:CYS:N   | 2.26                     | 0.65              |
| 1:1:3013:U:OP1    | 24:6:12:ARG:NE    | 2.30                     | 0.65              |
| 46:B:1772:U:P     | 61:Q:128:ARG:HH22 | 2.19                     | 0.65              |
| 55:K:11:ARG:O     | 58:N:133:LYS:NZ   | 2.29                     | 0.65              |
| 62:R:129:GLY:C    | 62:R:130:ARG:HD3  | 2.22                     | 0.65              |
| 1:AS:448:U:O2'    | 1:AS:483:U:OP1    | 2.15                     | 0.65              |
| 3:AU:79:A:O2'     | 36:CC:43:ARG:NH2  | 2.30                     | 0.65              |
| 28:BU:42:ILE:HD12 | 28:BU:98:SER:HB3  | 1.79                     | 0.65              |
| 46:CM:267:G:H2'   | 46:CM:268:C:C6    | 2.32                     | 0.65              |
| 46:CM:605:G:H5'   | 46:CM:611:G:N2    | 2.11                     | 0.65              |
| 1:1:662:U:H2'     | 1:1:663:A:H8      | 1.59                     | 0.65              |
| 1:1:2273:A:N3     | 1:1:2901:C:O2'    | 2.30                     | 0.65              |
| 51:G:175:PHE:HE2  | 51:G:198:ARG:HD2  | 1.62                     | 0.65              |
| 78:h:124:LYS:NZ   | 78:h:125:LYS:O    | 2.30                     | 0.65              |
| 78:h:190:LEU:HB3  | 78:h:191:LYS:HD2  | 1.79                     | 0.65              |
| 1:AS:93:G:H2'     | 1:AS:94:A:C8      | 2.32                     | 0.65              |
| 1:AS:3199:G:N2    | 1:AS:3218:U:O2    | 2.24                     | 0.65              |
| 2:AT:100:C:OP2    | 21:BN:52:LYS:NZ   | 2.30                     | 0.65              |
| 36:CC:83:LYS:HA   | 36:CC:89:ARG:HD3  | 1.79                     | 0.65              |
| 46:CM:947:C:H2'   | 46:CM:948:A:C8    | 2.32                     | 0.65              |
| 59:CZ:46:ARG:HD3  | 59:CZ:50:LYS:NZ   | 2.11                     | 0.65              |
| 79:DT:221:ASP:HB3 | 79:DT:226:LYS:HB3 | 1.79                     | 0.65              |
| 1:1:1106:U:H2'    | 1:1:1107:U:C6     | 2.31                     | 0.64              |
| 46:B:759:A:H61    | 46:B:770:C:H42    | 1.43                     | 0.64              |
| 46:B:1216:U:OP1   | 78:h:136:LYS:NZ   | 2.22                     | 0.64              |
| 46:B:1701:A:H2'   | 46:B:1702:A:H1'   | 1.78                     | 0.64              |
| 59:O:104:CYS:SG   | 59:O:115:VAL:HA   | 2.37                     | 0.64              |
| 11:BD:107:ASP:O   | 11:BD:109:GLN:NE2 | 2.29                     | 0.64              |
| 48:CO:130:SER:HB3 | 48:CO:179:CYS:C   | 2.21                     | 0.64              |
| 52:CS:145:ASP:OD1 | 52:CS:146:SER:N   | 2.30                     | 0.64              |
| 63:DD:21:VAL:HG22 | 63:DD:64:ILE:HG12 | 1.79                     | 0.64              |
| 81:P0:52:LEU:HB3  | 81:P0:86:PHE:HB2  | 1.78                     | 0.64              |
| 1:1:1593:C:P      | 35:AH:8:ARG:HH22  | 2.21                     | 0.64              |
| 1:1:2560:U:OP1    | 10:p:242:LYS:NZ   | 2.29                     | 0.64              |
| 46:B:778:U:O2'    | 46:B:779:U:O2     | 2.15                     | 0.64              |
| 1:AS:3260:A:H2'   | 1:AS:3261:A:C8    | 2.33                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:BD:92:PHE:HB2   | 11:BD:142:ASP:HB3  | 1.78                     | 0.64              |
| 36:CC:85:THR:HG23  | 36:CC:88:LEU:H     | 1.60                     | 0.64              |
| 48:CO:168:MET:HA   | 48:CO:197:ILE:HD12 | 1.78                     | 0.64              |
| 54:CU:75:ARG:O     | 54:CU:79:LYS:HG3   | 1.96                     | 0.64              |
| 60:DA:69:ASN:HB3   | 60:DA:73:ARG:HD2   | 1.79                     | 0.64              |
| 66:DG:117:SER:HB2  | 66:DG:123:ARG:HB2  | 1.79                     | 0.64              |
| 1:1:908:G:N7       | 4:j:9:ARG:NH2      | 2.45                     | 0.64              |
| 6:l:300:VAL:HB     | 19:y:39:ARG:HG2    | 1.78                     | 0.64              |
| 46:B:1463:G:H2'    | 46:B:1464:G:H8     | 1.63                     | 0.64              |
| 1:AS:662:U:H2'     | 1:AS:663:A:C8      | 2.32                     | 0.64              |
| 1:AS:3259:A:OP1    | 5:AX:128:LYS:NZ    | 2.21                     | 0.64              |
| 46:CM:850:A:H61    | 46:CM:948:A:H2     | 1.44                     | 0.64              |
| 46:CM:1485:G:H5''  | 66:DG:72:GLY:HA3   | 1.79                     | 0.64              |
| 48:CO:151:LYS:NZ   | 48:CO:153:THR:O    | 2.29                     | 0.64              |
| 53:CT:57:ASP:HA    | 53:CT:106:LEU:HA   | 1.79                     | 0.64              |
| 79:DT:19:TRP:HB2   | 79:DT:38:ARG:HD2   | 1.78                     | 0.64              |
| 1:1:1254:U:OP2     | 82:12:123:LYS:HE3  | 1.97                     | 0.64              |
| 1:1:2079:C:HO2'    | 1:1:2080:U:H6      | 1.45                     | 0.64              |
| 52:H:72:HIS:CD2    | 52:H:107:LYS:HD3   | 2.33                     | 0.64              |
| 1:AS:252:U:H5'     | 1:AS:253:A:H8      | 1.62                     | 0.64              |
| 1:AS:756:G:O2'     | 1:AS:766:G:N2      | 2.29                     | 0.64              |
| 1:AS:1115:C:H2'    | 1:AS:1116:A:C8     | 2.32                     | 0.64              |
| 75:DP:8:THR:O      | 75:DP:56:LEU:N     | 2.29                     | 0.64              |
| 1:1:2370:C:H1'     | 5:k:266:ARG:HH21   | 1.61                     | 0.64              |
| 1:1:3242:U:H2'     | 18:x:175:ARG:HH12  | 1.63                     | 0.64              |
| 57:M:31:LYS:NZ     | 57:M:36:ASP:OD1    | 2.23                     | 0.64              |
| 1:AS:628:A:H2'     | 1:AS:629:A:H8      | 1.63                     | 0.64              |
| 48:CO:66:PHE:HE2   | 61:DB:29:SER:CB    | 2.10                     | 0.64              |
| 48:CO:156:ALA:HB3  | 48:CO:161:LEU:HD21 | 1.80                     | 0.64              |
| 48:CO:220:GLN:NE2  | 48:CO:221:PRO:HD2  | 2.13                     | 0.64              |
| 1:1:1239:G:N2      | 1:1:1266:A:O2'     | 2.30                     | 0.64              |
| 28:AA:15:ARG:HD2   | 28:AA:79:HIS:CD2   | 2.33                     | 0.64              |
| 45:i:47:ASP:C      | 45:i:49:ALA:H      | 2.05                     | 0.64              |
| 50:F:124:LEU:HD11  | 50:F:153:TYR:HB3   | 1.80                     | 0.64              |
| 1:AS:3262:U:O4     | 5:AX:124:LYS:NZ    | 2.31                     | 0.64              |
| 46:CM:52:U:H2'     | 46:CM:53:G:C8      | 2.33                     | 0.64              |
| 52:CS:82:PHE:CE2   | 75:DP:49:ARG:HB2   | 2.32                     | 0.64              |
| 66:DG:7:ARG:NH2    | 66:DG:67:LEU:O     | 2.31                     | 0.64              |
| 79:DT:262:LEU:HD23 | 79:DT:265:ARG:NH1  | 2.13                     | 0.64              |
| 81:P0:56:ASN:ND2   | 81:P0:82:GLY:O     | 2.30                     | 0.64              |
| 1:1:498:C:H2'      | 1:1:499:G:C8       | 2.32                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:1020:G:H22    | 1:1:1023:A:H5''    | 1.62                     | 0.64              |
| 1:1:1632:C:OP1    | 28:AA:36:HIS:NE2   | 2.30                     | 0.64              |
| 1:1:2808:C:H5     | 1:1:2824:C:H42     | 1.46                     | 0.64              |
| 13:s:92:ARG:HD3   | 13:s:174:LYS:HE3   | 1.79                     | 0.64              |
| 46:B:12:U:H2'     | 46:B:13:C:C6       | 2.32                     | 0.64              |
| 25:BR:102:LYS:HE3 | 25:BR:105:ARG:HH22 | 1.61                     | 0.64              |
| 28:BU:57:MET:HG2  | 28:BU:61:LYS:HE2   | 1.79                     | 0.64              |
| 1:1:2912:A:OP2    | 5:k:2:SER:N        | 2.31                     | 0.64              |
| 10:p:144:ILE:HG23 | 10:p:176:VAL:HG21  | 1.80                     | 0.64              |
| 46:B:1460:G:H2'   | 46:B:1461:A:C8     | 2.33                     | 0.64              |
| 57:M:54:TYR:HD1   | 57:M:72:GLY:HA2    | 1.63                     | 0.64              |
| 1:AS:1617:A:H2'   | 1:AS:1618:U:C6     | 2.33                     | 0.64              |
| 1:AS:2520:A:H1'   | 1:AS:2521:C:C5     | 2.33                     | 0.64              |
| 46:CM:184:C:OP1   | 55:CV:152:ARG:NH2  | 2.29                     | 0.64              |
| 1:1:2669:A:H2'    | 1:1:2670:G:C8      | 2.33                     | 0.64              |
| 1:1:2669:A:H2'    | 1:1:2670:G:H8      | 1.63                     | 0.64              |
| 23:5:92:ILE:HD12  | 23:5:96:ILE:HD12   | 1.79                     | 0.64              |
| 45:i:90:ARG:HH21  | 46:B:1624:C:H2'    | 1.63                     | 0.64              |
| 46:B:31:C:OP1     | 70:Z:140:LYS:NZ    | 2.29                     | 0.64              |
| 46:B:221:U:O4     | 46:B:823:G:N2      | 2.31                     | 0.64              |
| 49:E:93:MET:HG3   | 49:E:116:VAL:HG23  | 1.78                     | 0.64              |
| 1:AS:1841:G:H5''  | 1:AS:1842:C:H5'    | 1.79                     | 0.64              |
| 2:AT:23:A:H2'     | 2:AT:24:A:C8       | 2.33                     | 0.64              |
| 46:CM:903:U:H2'   | 46:CM:904:A:C8     | 2.33                     | 0.64              |
| 59:CZ:105:GLN:CD  | 59:CZ:114:LYS:HB2  | 2.23                     | 0.64              |
| 72:DM:36:ALA:HB1  | 72:DM:38:HIS:HD2   | 1.63                     | 0.64              |
| 77:DR:50:THR:OG1  | 77:DR:53:LYS:HB2   | 1.97                     | 0.64              |
| 79:DT:6:VAL:HG22  | 79:DT:313:MET:HB3  | 1.80                     | 0.64              |
| 82:12:105:PRO:HD2 | 82:12:106:LEU:H    | 1.62                     | 0.64              |
| 1:1:976:A:H2'     | 1:1:977:U:H5'      | 1.78                     | 0.64              |
| 1:1:1255:A:N3     | 1:1:1276:C:O2'     | 2.29                     | 0.64              |
| 1:1:1600:A:H4'    | 1:1:1831:A:H4'     | 1.79                     | 0.64              |
| 46:B:1452:G:O2'   | 46:B:1589:C:OP1    | 2.16                     | 0.64              |
| 50:F:24:GLU:OE1   | 57:M:61:TRP:NE1    | 2.28                     | 0.64              |
| 54:J:5:ILE:HG22   | 54:J:7:SER:H       | 1.63                     | 0.64              |
| 1:AS:3317:U:H3'   | 55:CV:168:SER:HA   | 1.80                     | 0.64              |
| 3:AU:37:A:OP1     | 36:CC:89:ARG:NH2   | 2.30                     | 0.64              |
| 79:DT:112:LEU:N   | 79:DT:126:ALA:O    | 2.26                     | 0.64              |
| 1:1:1436:G:OP1    | 6:l:84:HIS:NE2     | 2.30                     | 0.63              |
| 45:i:115:LEU:O    | 45:i:118:GLU:HG3   | 1.97                     | 0.63              |
| 50:F:210:ALA:O    | 64:T:19:ARG:NH1    | 2.31                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:e:12:VAL:HG22   | 75:e:52:ASP:H      | 1.62                     | 0.63              |
| 1:AS:538:G:N2      | 1:AS:547:U:O2      | 2.26                     | 0.63              |
| 1:AS:1030:U:H2'    | 1:AS:1031:A:C8     | 2.34                     | 0.63              |
| 10:BC:242:LYS:O    | 10:BC:246:LYS:HG3  | 1.98                     | 0.63              |
| 46:CM:1254:U:H5'   | 46:CM:1418:U:OP2   | 1.98                     | 0.63              |
| 53:CT:234:LEU:HG   | 53:CT:235:LYS:HD3  | 1.80                     | 0.63              |
| 1:1:289:A:H2'      | 1:1:290:G:H8       | 1.64                     | 0.63              |
| 1:1:2932:C:H2'     | 1:1:2933:G:H8      | 1.64                     | 0.63              |
| 3:4:83:U:O2        | 27:9:51:ARG:NH2    | 2.31                     | 0.63              |
| 46:B:1:U:H1'       | 49:E:174:VAL:HG13  | 1.78                     | 0.63              |
| 65:U:69:ILE:HG22   | 65:U:73:MET:HE2    | 1.80                     | 0.63              |
| 79:AR:92:LEU:HB2   | 79:AR:104:PHE:HE1  | 1.63                     | 0.63              |
| 1:AS:254:A:O3'     | 36:CC:106:LYS:NZ   | 2.31                     | 0.63              |
| 1:AS:498:C:H5''    | 8:BA:25:ARG:NH2    | 2.13                     | 0.63              |
| 16:BI:183:THR:HG22 | 16:BI:187:ARG:HB2  | 1.80                     | 0.63              |
| 26:BS:47:GLN:NE2   | 26:BS:49:LYS:O     | 2.31                     | 0.63              |
| 46:CM:1275:U:H2'   | 46:CM:1276:G:C8    | 2.34                     | 0.63              |
| 48:CO:158:SER:O    | 48:CO:162:ARG:HG3  | 1.98                     | 0.63              |
| 79:DT:192:HIS:ND1  | 79:DT:214:ASP:OD2  | 2.31                     | 0.63              |
| 1:1:252:U:H5'      | 1:1:253:A:H8       | 1.62                     | 0.63              |
| 1:1:2210:A:N3      | 1:1:2406:U:O2'     | 2.31                     | 0.63              |
| 45:i:96:LYS:HG3    | 46:B:575:G:C4      | 2.32                     | 0.63              |
| 47:C:117:GLU:OE2   | 49:E:35:LYS:N      | 2.31                     | 0.63              |
| 5:AX:21:ARG:HE     | 5:AX:269:GLN:HG3   | 1.64                     | 0.63              |
| 20:BM:20:ARG:HH11  | 20:BM:21:LYS:HZ2   | 1.45                     | 0.63              |
| 46:CM:12:U:H2'     | 46:CM:13:C:C6      | 2.33                     | 0.63              |
| 51:CR:129:VAL:HG22 | 51:CR:139:VAL:HG22 | 1.81                     | 0.63              |
| 79:DT:6:VAL:CG2    | 79:DT:313:MET:HB3  | 2.27                     | 0.63              |
| 1:1:690:A:OP1      | 16:v:201:ARG:NH2   | 2.28                     | 0.63              |
| 12:r:82:ARG:NH1    | 12:r:83:ASP:OD1    | 2.32                     | 0.63              |
| 58:N:7:VAL:HG23    | 58:N:8:GLN:HG2     | 1.81                     | 0.63              |
| 1:AS:624:U:OP1     | 33:BZ:15:THR:OG1   | 2.16                     | 0.63              |
| 1:AS:2669:A:H2'    | 1:AS:2670:G:C8     | 2.34                     | 0.63              |
| 10:BC:231:ARG:NH1  | 37:CD:45:GLU:OE2   | 2.32                     | 0.63              |
| 80:BE:30:LYS:HG3   | 80:BE:63:GLU:HG3   | 1.79                     | 0.63              |
| 33:BZ:83:LEU:HD11  | 33:BZ:109:ILE:HG23 | 1.81                     | 0.63              |
| 45:CL:93:ARG:HG3   | 46:CM:1259:C:N3    | 2.14                     | 0.63              |
| 46:CM:1659:G:H2'   | 46:CM:1660:G:C8    | 2.33                     | 0.63              |
| 1:1:660:U:H2'      | 1:1:661:C:C6       | 2.34                     | 0.63              |
| 1:1:2932:C:H2'     | 1:1:2933:G:C8      | 2.32                     | 0.63              |
| 45:i:93:ARG:H      | 46:B:1259:C:H5     | 1.45                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:B:781:G:H4'     | 58:N:69:LYS:HZ1    | 1.64                     | 0.63              |
| 63:S:40:PRO:HB2    | 63:S:43:LEU:HB2    | 1.81                     | 0.63              |
| 1:AS:600:U:C2      | 1:AS:602:A:H1'     | 2.33                     | 0.63              |
| 1:AS:660:U:H2'     | 1:AS:661:C:C6      | 2.34                     | 0.63              |
| 1:AS:1591:U:O2'    | 1:AS:1602:U:O2     | 2.15                     | 0.63              |
| 1:AS:2738:U:H5'    | 83:AS:3401:3K5:H29 | 1.80                     | 0.63              |
| 19:BL:94:LEU:HD22  | 29:BV:119:PRO:HG3  | 1.81                     | 0.63              |
| 28:BU:73:LYS:HE3   | 28:BU:74:LEU:O     | 1.99                     | 0.63              |
| 39:CF:69:LEU:HD13  | 39:CF:70:PRO:O     | 1.99                     | 0.63              |
| 46:CM:518:A:H2'    | 46:CM:519:A:C8     | 2.34                     | 0.63              |
| 1:1:1234:C:H1'     | 82:12:139:VAL:HG13 | 1.80                     | 0.63              |
| 1:1:2649:G:O2'     | 1:1:2651:A:N1      | 2.28                     | 0.63              |
| 1:1:3133:G:H2'     | 1:1:3134:C:C6      | 2.33                     | 0.63              |
| 46:B:1719:A:H2'    | 46:B:1720:C:C6     | 2.34                     | 0.63              |
| 46:B:1750:A:H5''   | 46:B:1758:U:H5''   | 1.80                     | 0.63              |
| 49:E:134:ILE:HD13  | 49:E:186:ALA:HB1   | 1.80                     | 0.63              |
| 1:AS:2653:U:O2     | 13:BF:20:ASN:ND2   | 2.32                     | 0.63              |
| 35:CB:54:ILE:HD11  | 35:CB:78:GLY:HA2   | 1.81                     | 0.63              |
| 46:CM:226:G:H2'    | 46:CM:227:C:O4'    | 1.99                     | 0.63              |
| 48:CO:62:LYS:HD3   | 48:CO:91:VAL:HG12  | 1.80                     | 0.63              |
| 61:DB:79:ARG:HB3   | 61:DB:113:VAL:HG23 | 1.80                     | 0.63              |
| 68:DI:34:ILE:HG13  | 68:DI:69:LEU:HD11  | 1.81                     | 0.63              |
| 1:1:1794:A:H2'     | 1:1:1795:A:C8      | 2.34                     | 0.63              |
| 46:B:1543:A:OP1    | 62:R:115:TYR:OH    | 2.17                     | 0.63              |
| 1:AS:1755:U:H2'    | 1:AS:1756:A:H5''   | 1.80                     | 0.63              |
| 3:AU:52:A:H62      | 40:CG:27:ILE:HD13  | 1.63                     | 0.63              |
| 5:AX:142:LYS:HD3   | 5:AX:142:LYS:H     | 1.64                     | 0.63              |
| 26:BS:126:LEU:HD13 | 26:BS:135:ILE:HD12 | 1.81                     | 0.63              |
| 46:CM:405:A:H2'    | 46:CM:406:C:C6     | 2.34                     | 0.63              |
| 62:DC:24:ASP:O     | 62:DC:28:MET:HG3   | 1.98                     | 0.63              |
| 20:z:73:GLY:HA2    | 20:z:76:MET:HE2    | 1.80                     | 0.63              |
| 46:B:123:G:OP1     | 51:G:77:ARG:NH2    | 2.31                     | 0.63              |
| 46:B:1673:U:H2'    | 46:B:1674:U:O4'    | 1.99                     | 0.63              |
| 47:C:27:LYS:O      | 47:C:46:ASN:ND2    | 2.31                     | 0.63              |
| 59:O:129:ASP:O     | 59:O:131:ASP:N     | 2.31                     | 0.63              |
| 1:AS:1755:U:H3     | 1:AS:1762:G:H1     | 1.46                     | 0.63              |
| 1:AS:1795:A:H2'    | 1:AS:1796:A:C8     | 2.33                     | 0.63              |
| 47:CN:157:ASP:O    | 68:DI:66:ASP:HA    | 1.99                     | 0.63              |
| 49:CP:177:PRO:HG3  | 56:CW:17:ARG:HH12  | 1.64                     | 0.63              |
| 1:1:1115:C:H2'     | 1:1:1116:A:H8      | 1.64                     | 0.63              |
| 13:s:46:VAL:HG12   | 45:i:35:SER:HB3    | 1.80                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 68:X:15:ARG:NH1   | 68:X:33:GLN:OE1    | 2.31                     | 0.63              |
| 1:AS:92:C:OP2     | 1:AS:2736:C:O2'    | 2.13                     | 0.63              |
| 1:AS:208:A:H4'    | 1:AS:210:A:N7      | 2.14                     | 0.63              |
| 1:AS:2669:A:H2'   | 1:AS:2670:G:H8     | 1.63                     | 0.63              |
| 5:AX:58:ARG:HD2   | 5:AX:354:VAL:HG13  | 1.80                     | 0.63              |
| 46:CM:703:U:OP2   | 53:CT:234:LEU:HD13 | 1.99                     | 0.63              |
| 52:CS:117:ALA:O   | 52:CS:121:ILE:HG13 | 1.99                     | 0.63              |
| 70:DK:107:PHE:CD2 | 70:DK:114:LYS:HD3  | 2.34                     | 0.63              |
| 1:1:2184:G:H4'    | 1:1:2185:A:C8      | 2.34                     | 0.62              |
| 14:t:54:LEU:O     | 14:t:96:SER:OG     | 2.16                     | 0.62              |
| 45:i:104:GLN:HG3  | 45:i:109:GLN:NE2   | 2.14                     | 0.62              |
| 1:AS:3287:A:H2'   | 1:AS:3288:A:H8     | 1.62                     | 0.62              |
| 10:BC:154:ILE:O   | 10:BC:181:VAL:N    | 2.30                     | 0.62              |
| 15:BH:14:GLU:HB3  | 21:BN:149:LYS:HG2  | 1.81                     | 0.62              |
| 23:BP:68:VAL:HG12 | 23:BP:69:SER:H     | 1.61                     | 0.62              |
| 26:BS:141:TYR:HB3 | 36:CC:33:VAL:HG13  | 1.81                     | 0.62              |
| 54:CU:82:PRO:O    | 54:CU:84:ARG:N     | 2.31                     | 0.62              |
| 62:DC:1:MET:SD    | 62:DC:2:VAL:N      | 2.65                     | 0.62              |
| 64:DE:20:PHE:O    | 64:DE:24:LEU:HD12  | 1.98                     | 0.62              |
| 79:DT:103:ARG:HG2 | 79:DT:105:VAL:HG22 | 1.81                     | 0.62              |
| 79:DT:202:SER:OG  | 79:DT:204:ASP:OD1  | 2.14                     | 0.62              |
| 1:1:2126:U:H2'    | 1:1:2127:A:C8      | 2.34                     | 0.62              |
| 1:1:2632:G:OP1    | 1:1:2722:U:O2'     | 2.16                     | 0.62              |
| 1:1:3181:G:OP2    | 34:AG:2:ALA:N      | 2.32                     | 0.62              |
| 1:1:3196:U:H2'    | 1:1:3197:G:H8      | 1.65                     | 0.62              |
| 46:B:152:G:O6     | 71:a:128:ARG:NH2   | 2.31                     | 0.62              |
| 1:AS:480:G:H2'    | 1:AS:480:G:N3      | 2.12                     | 0.62              |
| 1:AS:1692:A:H2'   | 1:AS:1693:A:C8     | 2.34                     | 0.62              |
| 1:AS:1747:G:H5'   | 39:CF:26:LYS:HE2   | 1.79                     | 0.62              |
| 16:BI:31:ARG:NH1  | 16:BI:124:ASP:OD2  | 2.31                     | 0.62              |
| 28:BU:3:LYS:HE3   | 28:BU:30:ASP:OD2   | 1.99                     | 0.62              |
| 39:CF:63:LYS:O    | 39:CF:67:GLN:HG3   | 1.99                     | 0.62              |
| 46:CM:1219:A:O2'  | 78:DS:187:HIS:CG   | 2.52                     | 0.62              |
| 54:CU:92:ARG:CZ   | 54:CU:120:LYS:HB3  | 2.29                     | 0.62              |
| 54:CU:134:LYS:C   | 54:CU:135:ARG:HD2  | 2.24                     | 0.62              |
| 79:DT:128:ARG:HG2 | 79:DT:151:TRP:CD2  | 2.35                     | 0.62              |
| 81:P0:25:ILE:HD13 | 81:P0:89:THR:HG22  | 1.80                     | 0.62              |
| 1:1:2709:C:O2'    | 30:AC:36:ASP:OD1   | 2.15                     | 0.62              |
| 12:r:54:SER:OG    | 12:r:130:SER:O     | 2.17                     | 0.62              |
| 46:B:184:C:OP1    | 55:K:152:ARG:NH2   | 2.29                     | 0.62              |
| 46:B:216:A:H4'    | 46:B:217:A:OP1     | 2.00                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:I:57:ASP:HA     | 53:I:106:LEU:HA    | 1.81                     | 0.62              |
| 79:AR:202:SER:OG   | 79:AR:204:ASP:OD1  | 2.17                     | 0.62              |
| 1:AS:307:A:H2'     | 1:AS:308:A:C8      | 2.34                     | 0.62              |
| 28:BU:76:ASN:ND2   | 28:BU:78:ASN:HB2   | 2.15                     | 0.62              |
| 46:CM:142:G:O2'    | 46:CM:143:A:O5'    | 2.18                     | 0.62              |
| 46:CM:1214:G:N1    | 59:CZ:47:GLU:OE2   | 2.28                     | 0.62              |
| 46:CM:1215:A:OP2   | 78:DS:139:LYS:HD2  | 1.99                     | 0.62              |
| 81:P0:64:ARG:HA    | 81:P0:77:LEU:HD11  | 1.81                     | 0.62              |
| 1:1:244:G:O3'      | 14:BG:134:GLU:HB2  | 1.99                     | 0.62              |
| 21:0:99:ARG:NH1    | 21:0:126:VAL:O     | 2.32                     | 0.62              |
| 1:AS:252:U:H5'     | 1:AS:253:A:C8      | 2.33                     | 0.62              |
| 1:AS:739:C:N3      | 19:BL:141:ARG:NH2  | 2.47                     | 0.62              |
| 1:AS:3136:C:H2'    | 1:AS:3137:A:H8     | 1.64                     | 0.62              |
| 46:CM:1668:A:H8    | 53:CT:65:GLN:HG3   | 1.63                     | 0.62              |
| 79:DT:82:LEU:HD21  | 79:DT:104:PHE:CE2  | 2.33                     | 0.62              |
| 79:DT:137:THR:HG22 | 79:DT:137:THR:O    | 1.99                     | 0.62              |
| 1:1:628:A:H2'      | 1:1:629:A:H8       | 1.62                     | 0.62              |
| 18:x:32:THR:HG21   | 18:x:87:SER:HB3    | 1.81                     | 0.62              |
| 46:B:829:A:H2'     | 46:B:830:G:C8      | 2.34                     | 0.62              |
| 46:B:1238:U:H5''   | 78:h:172:ILE:HD12  | 1.81                     | 0.62              |
| 46:B:1410:A:H2'    | 49:E:87:ALA:HB3    | 1.81                     | 0.62              |
| 57:M:55:VAL:HG12   | 57:M:68:LEU:HA     | 1.80                     | 0.62              |
| 59:O:29:LYS:HE2    | 59:O:100:TRP:CE3   | 2.33                     | 0.62              |
| 79:AR:102:GLN:NE2  | 79:AR:103:ARG:O    | 2.33                     | 0.62              |
| 1:AS:1018:U:H2'    | 1:AS:1019:U:H5''   | 1.82                     | 0.62              |
| 10:BC:94:LEU:HD21  | 10:BC:212:LEU:HD12 | 1.80                     | 0.62              |
| 14:BG:178:GLU:O    | 14:BG:182:LYS:HB2  | 2.00                     | 0.62              |
| 23:BP:28:PHE:HE1   | 23:BP:33:TYR:HB2   | 1.62                     | 0.62              |
| 46:CM:91:G:OP1     | 46:CM:395:A:N6     | 2.32                     | 0.62              |
| 46:CM:702:G:H4'    | 46:CM:703:U:OP1    | 1.98                     | 0.62              |
| 48:CO:24:PHE:HE2   | 61:DB:65:LYS:HE3   | 1.63                     | 0.62              |
| 70:DK:30:LYS:HE2   | 70:DK:34:LEU:HD11  | 1.82                     | 0.62              |
| 1:1:483:U:H2'      | 1:1:484:U:C6       | 2.34                     | 0.62              |
| 1:1:1519:U:H5'     | 26:8:113:LEU:HD13  | 1.79                     | 0.62              |
| 1:1:1795:A:H2'     | 1:1:1796:A:C8      | 2.34                     | 0.62              |
| 1:1:2717:G:N2      | 1:1:2720:A:OP2     | 2.25                     | 0.62              |
| 1:1:3254:G:H2'     | 1:1:3255:G:C8      | 2.34                     | 0.62              |
| 1:1:3344:U:H4'     | 5:k:315:GLY:HA2    | 1.80                     | 0.62              |
| 46:B:767:G:HO2'    | 46:B:768:C:H6      | 1.47                     | 0.62              |
| 46:B:1615:U:H2'    | 46:B:1616:G:C8     | 2.35                     | 0.62              |
| 1:AS:1663:A:H2'    | 1:AS:1664:G:H8     | 1.63                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AU:83:U:O2      | 27:BT:51:ARG:NH2   | 2.33                     | 0.62              |
| 16:BI:11:GLN:O    | 16:BI:14:LYS:NZ    | 2.28                     | 0.62              |
| 23:BP:87:LEU:HD13 | 23:BP:92:ILE:HG13  | 1.82                     | 0.62              |
| 37:CD:61:ARG:NH2  | 37:CD:93:ILE:HG23  | 2.14                     | 0.62              |
| 46:CM:78:A:H2     | 53:CT:174:LYS:HG3  | 1.64                     | 0.62              |
| 46:CM:794:G:N3    | 54:CU:104:LYS:NZ   | 2.47                     | 0.62              |
| 48:CO:48:ILE:HG21 | 48:CO:61:LEU:HD22  | 1.81                     | 0.62              |
| 62:DC:33:PHE:HA   | 62:DC:36:LEU:HD21  | 1.81                     | 0.62              |
| 1:1:1692:A:H2'    | 1:1:1693:A:C8      | 2.35                     | 0.62              |
| 46:B:681:C:H3'    | 46:B:682:A:C8      | 2.35                     | 0.62              |
| 47:C:47:ILE:HD12  | 64:T:106:THR:HG22  | 1.81                     | 0.62              |
| 1:AS:1199:A:H2'   | 1:AS:1200:A:C8     | 2.35                     | 0.62              |
| 1:AS:2535:A:OP1   | 4:AW:69:TYR:OH     | 2.14                     | 0.62              |
| 10:BC:221:ALA:O   | 10:BC:226:LYS:HB2  | 1.99                     | 0.62              |
| 14:BG:59:ARG:NH1  | 14:BG:68:LYS:O     | 2.33                     | 0.62              |
| 26:BS:141:TYR:O   | 26:BS:142:ILE:HG13 | 2.00                     | 0.62              |
| 46:CM:542:A:H4'   | 77:DR:28:LYS:HZ2   | 1.65                     | 0.62              |
| 46:CM:671:G:H5'   | 46:CM:672:U:OP2    | 1.99                     | 0.62              |
| 46:CM:970:G:H2'   | 46:CM:971:G:C8     | 2.34                     | 0.62              |
| 59:CZ:63:CYS:SG   | 59:CZ:64:ASP:N     | 2.73                     | 0.62              |
| 64:DE:78:ARG:HH11 | 64:DE:81:LYS:HD3   | 1.63                     | 0.62              |
| 50:F:214:ASP:OD1  | 50:F:215:GLU:N     | 2.19                     | 0.62              |
| 55:K:2:GLY:O      | 55:K:24:LYS:NZ     | 2.18                     | 0.62              |
| 56:L:108:ARG:NH1  | 56:L:110:GLN:OE1   | 2.31                     | 0.62              |
| 60:P:45:LEU:HB3   | 60:P:49:GLN:HB2    | 1.80                     | 0.62              |
| 70:Z:107:PHE:HE2  | 70:Z:114:LYS:HD3   | 1.64                     | 0.62              |
| 1:AS:538:G:H2'    | 1:AS:539:G:C8      | 2.35                     | 0.62              |
| 5:AX:137:TYR:HA   | 5:AX:141:ALA:HB2   | 1.82                     | 0.62              |
| 27:BT:51:ARG:HG2  | 27:BT:52:GLN:H     | 1.64                     | 0.62              |
| 28:BU:100:ALA:HA  | 28:BU:106:GLN:HB3  | 1.82                     | 0.62              |
| 46:CM:217:A:C8    | 46:CM:816:U:O2     | 2.53                     | 0.62              |
| 55:CV:139:ALA:HB3 | 55:CV:141:ARG:NH1  | 2.14                     | 0.62              |
| 1:1:365:A:OP1     | 6:l:85:ARG:NH1     | 2.32                     | 0.62              |
| 1:1:2206:A:H2'    | 1:1:2207:A:C8      | 2.35                     | 0.62              |
| 10:p:222:ASN:HA   | 10:p:226:LYS:HE2   | 1.81                     | 0.62              |
| 45:i:71:LYS:HB3   | 46:B:1446:A:H4'    | 1.81                     | 0.62              |
| 46:B:213:A:H2'    | 46:B:214:U:H5'     | 1.82                     | 0.62              |
| 46:B:589:A:P      | 77:g:43:ARG:HH22   | 2.23                     | 0.62              |
| 46:B:869:A:H62    | 46:B:913:U:H3      | 1.45                     | 0.62              |
| 1:AS:1782:G:H2'   | 1:AS:1783:A:C8     | 2.35                     | 0.62              |
| 4:AW:6:ARG:HH12   | 4:AW:199:THR:H     | 1.46                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:BD:110:ASP:HB3  | 11:BD:128:ILE:HD12 | 1.82                     | 0.62              |
| 53:CT:10:ASN:ND2   | 53:CT:127:THR:O    | 2.26                     | 0.62              |
| 70:DK:69:ARG:HG3   | 70:DK:117:ILE:HG12 | 1.80                     | 0.62              |
| 1:1:2720:A:H1'     | 7:m:36:LEU:HD23    | 1.82                     | 0.62              |
| 46:B:1193:A:H4'    | 46:B:1255:G:P      | 2.40                     | 0.62              |
| 1:AS:289:A:H2'     | 1:AS:290:G:H8      | 1.65                     | 0.62              |
| 1:AS:1473:A:OP1    | 1:AS:3047:G:O2'    | 2.17                     | 0.62              |
| 1:AS:2220:A:H5''   | 4:AW:244:GLY:HA3   | 1.82                     | 0.62              |
| 1:AS:2832:U:O2     | 1:AS:2910:G:H4'    | 2.00                     | 0.62              |
| 1:AS:2988:A:H2'    | 1:AS:2989:A:H8     | 1.65                     | 0.62              |
| 20:BM:30:THR:O     | 20:BM:34:ASN:ND2   | 2.31                     | 0.62              |
| 46:CM:1578:C:H2'   | 46:CM:1579:A:H8    | 1.65                     | 0.62              |
| 48:CO:90:GLU:OE2   | 48:CO:96:LEU:HA    | 2.00                     | 0.62              |
| 57:CX:12:HIS:HB3   | 57:CX:80:LEU:HD21  | 1.80                     | 0.62              |
| 59:CZ:46:ARG:O     | 59:CZ:50:LYS:HG3   | 2.00                     | 0.62              |
| 59:CZ:137:LEU:O    | 59:CZ:141:SER:N    | 2.33                     | 0.62              |
| 4:j:77:ILE:HD13    | 4:j:128:ARG:HB3    | 1.82                     | 0.61              |
| 15:u:14:GLU:HB3    | 21:0:149:LYS:HG2   | 1.81                     | 0.61              |
| 59:O:52:LEU:HD21   | 59:O:60:CYS:SG     | 2.39                     | 0.61              |
| 1:AS:16:G:H4'      | 36:CC:75:TYR:CZ    | 2.35                     | 0.61              |
| 1:AS:527:G:H2'     | 1:AS:528:A:C8      | 2.35                     | 0.61              |
| 14:BG:59:ARG:NH2   | 14:BG:152:PRO:HG2  | 2.14                     | 0.61              |
| 46:CM:586:U:OP2    | 77:DR:26:LYS:NZ    | 2.33                     | 0.61              |
| 46:CM:1241:A:H5'   | 46:CM:1242:U:H6    | 1.64                     | 0.61              |
| 61:DB:52:PRO:HB3   | 61:DB:95:SER:OG    | 2.00                     | 0.61              |
| 64:DE:75:GLU:HG3   | 64:DE:76:GLU:OE1   | 2.00                     | 0.61              |
| 65:DF:4:VAL:N      | 72:DM:82:GLN:OE1   | 2.32                     | 0.61              |
| 68:DI:36:ILE:HD12  | 68:DI:78:LEU:HD13  | 1.81                     | 0.61              |
| 78:DS:182:TYR:HH   | 78:DS:187:HIS:CE1  | 2.18                     | 0.61              |
| 79:DT:107:HIS:HA   | 79:DT:133:LYS:HE3  | 1.82                     | 0.61              |
| 82:12:103:ASN:HB3  | 82:12:105:PRO:HD3  | 1.82                     | 0.61              |
| 1:1:498:C:H2'      | 1:1:499:G:H8       | 1.64                     | 0.61              |
| 1:1:618:U:H2'      | 18:x:167:ARG:NH1   | 2.15                     | 0.61              |
| 46:B:317:U:H4'     | 46:B:321:A:C8      | 2.34                     | 0.61              |
| 46:B:944:U:O2      | 60:P:61:SER:OG     | 2.18                     | 0.61              |
| 50:CQ:219:ILE:O    | 79:DT:191:GLY:HA2  | 2.00                     | 0.61              |
| 50:CQ:223:THR:HG21 | 79:DT:225:ASN:HB3  | 1.82                     | 0.61              |
| 52:CS:100:ASN:O    | 52:CS:102:ARG:N    | 2.33                     | 0.61              |
| 69:DJ:81:VAL:O     | 69:DJ:122:SER:OG   | 2.11                     | 0.61              |
| 1:1:1691:U:O2'     | 1:1:1745:A:N1      | 2.33                     | 0.61              |
| 68:X:55:LEU:HD11   | 68:X:69:LEU:HD21   | 1.81                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BU:42:ILE:CD1  | 28:BU:98:SER:HA    | 2.31                     | 0.61              |
| 39:CF:9:LYS:O     | 39:CF:13:GLU:HG2   | 2.00                     | 0.61              |
| 45:CL:61:GLU:O    | 45:CL:63:ALA:N     | 2.32                     | 0.61              |
| 52:CS:58:LEU:HD13 | 52:CS:168:VAL:HG22 | 1.83                     | 0.61              |
| 79:DT:88:ARG:HG2  | 79:DT:109:GLY:C    | 2.25                     | 0.61              |
| 15:u:14:GLU:HG2   | 15:u:17:ARG:HG2    | 1.82                     | 0.61              |
| 46:B:878:U:H5'    | 46:B:879:U:OP2     | 2.00                     | 0.61              |
| 10:BC:62:GLN:HE22 | 10:BC:66:LEU:HB2   | 1.65                     | 0.61              |
| 36:CC:47:VAL:O    | 36:CC:51:ILE:HG13  | 2.00                     | 0.61              |
| 41:CH:23:CYS:HB2  | 41:CH:38:LYS:HD2   | 1.82                     | 0.61              |
| 46:CM:405:A:H2'   | 46:CM:406:C:H6     | 1.66                     | 0.61              |
| 46:CM:1145:A:H2'  | 46:CM:1146:C:H6    | 1.64                     | 0.61              |
| 46:CM:1301:G:OP1  | 64:DE:7:LYS:N      | 2.30                     | 0.61              |
| 1:1:2254:G:OP1    | 42:AO:16:LYS:NZ    | 2.34                     | 0.61              |
| 2:3:23:A:H2'      | 2:3:24:A:C8        | 2.35                     | 0.61              |
| 16:v:159:ARG:HB2  | 16:v:164:LEU:HB2   | 1.81                     | 0.61              |
| 20:z:176:ARG:NH1  | 46:B:837:C:OP1     | 2.34                     | 0.61              |
| 23:5:53:ASP:HA    | 23:5:69:SER:HB3    | 1.81                     | 0.61              |
| 32:AE:45:THR:HG22 | 32:AE:47:ASP:H     | 1.65                     | 0.61              |
| 43:AP:15:LYS:HD3  | 43:AP:18:ARG:HH21  | 1.65                     | 0.61              |
| 46:B:1527:G:OP2   | 65:U:40:ARG:NH2    | 2.33                     | 0.61              |
| 49:E:138:TYR:OH   | 49:E:144:GLY:O     | 2.13                     | 0.61              |
| 14:BG:168:ALA:N   | 29:BV:135:GLU:OE2  | 2.33                     | 0.61              |
| 17:BJ:63:THR:HG21 | 17:BJ:69:LYS:HB2   | 1.81                     | 0.61              |
| 46:CM:1276:G:H22  | 46:CM:1309:G:N2    | 1.98                     | 0.61              |
| 46:CM:1457:A:H2   | 46:CM:1460:G:N3    | 1.98                     | 0.61              |
| 46:CM:1579:A:H2'  | 46:CM:1580:A:C8    | 2.36                     | 0.61              |
| 59:CZ:46:ARG:HD3  | 59:CZ:50:LYS:HZ1   | 1.64                     | 0.61              |
| 59:CZ:81:GLU:H    | 59:CZ:82:PRO:HD2   | 1.64                     | 0.61              |
| 59:CZ:128:ALA:HB1 | 59:CZ:132:GLU:HB2  | 1.81                     | 0.61              |
| 1:1:428:U:H2'     | 1:1:429:U:C6       | 2.36                     | 0.61              |
| 1:1:1020:G:N2     | 1:1:1023:A:H5''    | 2.14                     | 0.61              |
| 1:1:1130:G:O2'    | 1:1:2614:A:N3      | 2.29                     | 0.61              |
| 1:1:2740:U:H2'    | 1:1:2741:A:H8      | 1.64                     | 0.61              |
| 1:1:3136:C:H2'    | 1:1:3137:A:C8      | 2.35                     | 0.61              |
| 38:AK:25:ARG:NH1  | 40:AM:50:GLY:HA2   | 2.16                     | 0.61              |
| 45:i:80:ALA:HB2   | 46:B:1163:G:H21    | 1.66                     | 0.61              |
| 46:B:1579:A:H2'   | 46:B:1580:A:C8     | 2.35                     | 0.61              |
| 57:M:14:TYR:HD2   | 57:M:21:VAL:HG22   | 1.64                     | 0.61              |
| 62:R:121:ILE:HG23 | 62:R:123:TYR:N     | 2.16                     | 0.61              |
| 1:AS:1011:C:H4'   | 1:AS:1012:U:H6     | 1.65                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:2115:U:OP2    | 1:AS:2120:A:N6     | 2.25                     | 0.61              |
| 10:BC:70:LEU:HD23  | 10:BC:71:LYS:H     | 1.65                     | 0.61              |
| 48:CO:97:LEU:HD21  | 48:CO:228:LEU:HD21 | 1.83                     | 0.61              |
| 48:CO:185:THR:O    | 48:CO:189:ILE:HG13 | 2.00                     | 0.61              |
| 79:DT:113:SER:HB3  | 79:DT:154:ALA:HA   | 1.81                     | 0.61              |
| 1:1:1278:G:OP1     | 81:P0:55:LYS:HG3   | 2.00                     | 0.61              |
| 1:1:2163:G:O2'     | 1:1:2292:U:OP2     | 2.19                     | 0.61              |
| 11:q:47:LYS:HB2    | 15:u:5:VAL:HB      | 1.81                     | 0.61              |
| 46:B:515:U:H2'     | 46:B:516:A:H8      | 1.64                     | 0.61              |
| 46:B:1701:A:H2'    | 46:B:1702:A:C1'    | 2.31                     | 0.61              |
| 46:B:1741:A:C5     | 86:B:1851:GET:H21  | 2.36                     | 0.61              |
| 70:Z:69:ARG:HG3    | 70:Z:117:ILE:HG12  | 1.83                     | 0.61              |
| 1:AS:496:A:H2'     | 1:AS:497:U:C6      | 2.35                     | 0.61              |
| 20:BM:134:HIS:CE1  | 20:BM:136:ARG:HB3  | 2.36                     | 0.61              |
| 46:CM:140:U:OP2    | 53:CT:139:ASN:ND2  | 2.32                     | 0.61              |
| 46:CM:216:A:N6     | 46:CM:829:A:O2'    | 2.34                     | 0.61              |
| 46:CM:1218:G:N2    | 46:CM:1238:U:H1'   | 2.16                     | 0.61              |
| 46:CM:1663:U:H5''  | 55:CV:58:LEU:HD21  | 1.83                     | 0.61              |
| 65:DF:67:GLU:HA    | 65:DF:70:VAL:HG22  | 1.83                     | 0.61              |
| 1:1:2116:A:C4      | 38:AK:3:LYS:HB3    | 2.35                     | 0.61              |
| 1:1:2587:G:H2'     | 1:1:2588:C:H6      | 1.64                     | 0.61              |
| 46:B:1668:A:H1'    | 53:I:66:GLY:HA2    | 1.81                     | 0.61              |
| 1:AS:907:C:OP1     | 4:AW:14:SER:OG     | 2.19                     | 0.61              |
| 1:AS:1004:U:O2'    | 80:BE:35:ASP:OD2   | 2.19                     | 0.61              |
| 21:BN:42:TRP:O     | 21:BN:46:GLN:HG3   | 2.00                     | 0.61              |
| 27:BT:106:ILE:HG21 | 27:BT:109:LEU:HD23 | 1.83                     | 0.61              |
| 31:BX:59:GLU:OE1   | 31:BX:71:TYR:OH    | 2.18                     | 0.61              |
| 36:CC:40:SER:C     | 36:CC:42:PRO:HD3   | 2.25                     | 0.61              |
| 46:CM:16:G:H2'     | 46:CM:17:C:C6      | 2.36                     | 0.61              |
| 46:CM:857:G:N2     | 46:CM:1032:G:H4'   | 2.16                     | 0.61              |
| 46:CM:1460:G:H2'   | 46:CM:1461:A:C8    | 2.36                     | 0.61              |
| 46:CM:1520:C:OP2   | 72:DM:77:ARG:NH1   | 2.31                     | 0.61              |
| 49:CP:171:LYS:HE2  | 56:CW:57:ARG:CZ    | 2.31                     | 0.61              |
| 55:CV:78:ILE:HG21  | 55:CV:96:LEU:HD21  | 1.82                     | 0.61              |
| 75:DP:19:THR:HG23  | 75:DP:25:VAL:HG13  | 1.83                     | 0.61              |
| 79:DT:240:LEU:HD23 | 79:DT:251:ALA:HB2  | 1.83                     | 0.61              |
| 79:DT:254:THR:O    | 79:DT:282:LYS:HE2  | 2.00                     | 0.61              |
| 1:1:679:U:O2'      | 1:1:695:G:O6       | 2.17                     | 0.61              |
| 1:1:907:C:H42      | 4:j:3:ARG:HD3      | 1.66                     | 0.61              |
| 1:1:1014:G:H1      | 1:1:1030:U:H3      | 1.49                     | 0.61              |
| 1:1:2196:G:H2'     | 1:1:2197:A:H8      | 1.66                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:2789:A:H4'    | 1:1:2790:U:OP2     | 2.00                     | 0.61              |
| 8:n:65:SER:HB2    | 8:n:75:LEU:HD23    | 1.82                     | 0.61              |
| 15:u:20:LEU:HD21  | 15:u:23:ASN:HA     | 1.83                     | 0.61              |
| 29:AB:36:GLY:HA3  | 29:AB:40:HIS:CE1   | 2.35                     | 0.61              |
| 46:B:269:A:H5'    | 46:B:270:U:OP2     | 2.00                     | 0.61              |
| 49:E:233:SER:HB3  | 49:E:236:GLU:HG3   | 1.83                     | 0.61              |
| 1:AS:820:C:H5''   | 4:AW:21:ARG:HD3    | 1.83                     | 0.61              |
| 1:AS:1481:G:N2    | 35:CB:4:ARG:HD2    | 2.15                     | 0.61              |
| 37:CD:88:GLU:HB3  | 37:CD:89:MET:HE2   | 1.82                     | 0.61              |
| 39:CF:36:LYS:HG2  | 39:CF:37:LYS:HG3   | 1.83                     | 0.61              |
| 46:CM:1543:A:OP1  | 62:DC:115:TYR:OH   | 2.17                     | 0.61              |
| 46:CM:1719:A:H2'  | 46:CM:1720:C:C6    | 2.36                     | 0.61              |
| 48:CO:70:LEU:CD2  | 48:CO:79:HIS:HD2   | 2.14                     | 0.61              |
| 79:DT:46:LYS:O    | 79:DT:56:GLY:HA2   | 2.01                     | 0.61              |
| 1:1:1923:G:C8     | 44:AQ:16:VAL:HG12  | 2.36                     | 0.61              |
| 1:1:2668:A:H2'    | 1:1:2669:A:C8      | 2.36                     | 0.61              |
| 1:1:2675:A:N6     | 7:m:28:THR:O       | 2.34                     | 0.61              |
| 63:S:30:ILE:HG12  | 63:S:35:ILE:HG22   | 1.83                     | 0.61              |
| 65:U:24:GLY:HA2   | 65:U:58:ALA:HB3    | 1.83                     | 0.61              |
| 1:AS:2139:G:H5''  | 4:AW:227:ARG:HH12  | 1.66                     | 0.61              |
| 46:CM:1:U:OP2     | 56:CW:57:ARG:NH2   | 2.34                     | 0.61              |
| 46:CM:1719:A:H2'  | 46:CM:1720:C:H6    | 1.66                     | 0.61              |
| 81:P0:73:PHE:HB3  | 81:P0:76:LEU:HB2   | 1.82                     | 0.61              |
| 1:1:168:U:OP1     | 14:t:128:LYS:NZ    | 2.34                     | 0.60              |
| 1:1:2645:A:OP1    | 13:s:95:ASN:ND2    | 2.34                     | 0.60              |
| 1:1:2855:U:H2'    | 1:1:2856:C:C6      | 2.36                     | 0.60              |
| 1:1:2899:C:H2'    | 1:1:2900:C:C6      | 2.36                     | 0.60              |
| 3:4:75:G:OP2      | 27:9:74:TYR:OH     | 2.18                     | 0.60              |
| 46:B:91:G:OP1     | 46:B:395:A:N6      | 2.32                     | 0.60              |
| 46:B:1592:G:OP2   | 63:S:126:LYS:NZ    | 2.32                     | 0.60              |
| 79:AR:76:ALA:HB3  | 79:AR:120:LEU:HD11 | 1.82                     | 0.60              |
| 1:AS:431:A:H2'    | 1:AS:432:G:H8      | 1.66                     | 0.60              |
| 1:AS:1345:G:N2    | 6:AY:292:ASN:O     | 2.33                     | 0.60              |
| 10:BC:62:GLN:HG2  | 16:BI:28:TRP:HZ2   | 1.66                     | 0.60              |
| 14:BG:155:GLU:OE2 | 29:BV:126:LYS:NZ   | 2.18                     | 0.60              |
| 39:CF:42:LYS:HG2  | 39:CF:55:VAL:HG22  | 1.82                     | 0.60              |
| 1:1:1857:G:O2'    | 1:1:3038:U:OP1     | 2.18                     | 0.60              |
| 1:1:2210:A:H2'    | 1:1:2211:A:C8      | 2.36                     | 0.60              |
| 26:8:34:LEU:HD12  | 26:8:35:PRO:HD2    | 1.83                     | 0.60              |
| 45:i:113:ARG:O    | 45:i:114:GLU:C     | 2.44                     | 0.60              |
| 46:B:1130:U:O2'   | 49:E:84:GLN:O      | 2.18                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:1468:C:H5''  | 46:B:1508:G:H22    | 1.66                     | 0.60              |
| 79:AR:302:TYR:CE2 | 79:AR:308:ARG:HD2  | 2.36                     | 0.60              |
| 1:AS:128:C:OP1    | 26:BS:45:LYS:NZ    | 2.34                     | 0.60              |
| 1:AS:2210:A:H2'   | 1:AS:2211:A:C8     | 2.36                     | 0.60              |
| 30:BW:16:ALA:HB1  | 30:BW:21:ILE:HD11  | 1.82                     | 0.60              |
| 54:CU:158:VAL:C   | 54:CU:160:TYR:H    | 2.09                     | 0.60              |
| 78:DS:186:CYS:SG  | 78:DS:188:LEU:HD22 | 2.41                     | 0.60              |
| 79:DT:90:LEU:HD11 | 79:DT:125:SER:OG   | 2.01                     | 0.60              |
| 1:1:169:G:H1      | 1:1:248:U:H3       | 1.46                     | 0.60              |
| 1:1:2322:U:H2'    | 1:1:2323:A:C8      | 2.37                     | 0.60              |
| 1:1:2535:A:OP1    | 4:j:69:TYR:OH      | 2.16                     | 0.60              |
| 62:R:77:LYS:HB3   | 62:R:102:PHE:CE1   | 2.36                     | 0.60              |
| 75:e:12:VAL:HG12  | 75:e:30:VAL:HG12   | 1.83                     | 0.60              |
| 1:AS:273:A:H2'    | 1:AS:274:G:H8      | 1.65                     | 0.60              |
| 1:AS:487:C:O2'    | 1:AS:488:G:OP1     | 2.18                     | 0.60              |
| 23:BP:18:ASP:OD2  | 23:BP:63:LYS:NZ    | 2.34                     | 0.60              |
| 28:BU:54:THR:OG1  | 28:BU:57:MET:HG3   | 2.02                     | 0.60              |
| 45:CL:42:ALA:O    | 45:CL:44:ALA:N     | 2.34                     | 0.60              |
| 46:CM:3:U:O2      | 56:CW:17:ARG:NH2   | 2.34                     | 0.60              |
| 46:CM:1237:C:H1'  | 78:DS:182:TYR:HD2  | 1.64                     | 0.60              |
| 54:CU:47:VAL:HG23 | 54:CU:48:ASN:N     | 2.16                     | 0.60              |
| 59:CZ:40:GLY:O    | 59:CZ:123:VAL:HA   | 2.00                     | 0.60              |
| 73:DN:26:CYS:HB3  | 73:DN:77:CYS:SG    | 2.40                     | 0.60              |
| 1:1:212:A:OP1     | 27:9:2:ALA:N       | 2.34                     | 0.60              |
| 1:1:756:G:O2'     | 1:1:766:G:N2       | 2.32                     | 0.60              |
| 1:1:1672:A:O2'    | 23:5:103:GLN:OE1   | 2.20                     | 0.60              |
| 1:1:2070:A:O2'    | 20:z:114:LYS:NZ    | 2.24                     | 0.60              |
| 2:3:65:G:O3'      | 12:r:204:GLY:HA2   | 2.00                     | 0.60              |
| 15:u:17:ARG:HD2   | 15:u:61:VAL:HG22   | 1.83                     | 0.60              |
| 18:x:4:TYR:CZ     | 18:x:18:ARG:HG3    | 2.36                     | 0.60              |
| 46:B:826:U:H2'    | 46:B:827:C:O4'     | 2.00                     | 0.60              |
| 62:R:97:TYR:HE1   | 62:R:102:PHE:CZ    | 2.20                     | 0.60              |
| 64:T:71:PHE:HD1   | 64:T:72:LYS:H      | 1.48                     | 0.60              |
| 1:AS:479:C:H2'    | 1:AS:480:G:H8      | 1.67                     | 0.60              |
| 10:BC:69:ARG:HD3  | 10:BC:238:ILE:O    | 2.01                     | 0.60              |
| 17:w:131:LYS:HB3  | 17:w:134:ARG:HG2   | 1.82                     | 0.60              |
| 27:9:116:LYS:HE2  | 27:9:126:ALA:HB1   | 1.83                     | 0.60              |
| 46:B:157:U:H5'    | 71:a:117:LYS:HB3   | 1.84                     | 0.60              |
| 46:B:1219:A:O2'   | 78:h:187:HIS:ND1   | 2.33                     | 0.60              |
| 1:AS:2503:G:OP2   | 4:AW:37:ARG:NH2    | 2.34                     | 0.60              |
| 1:AS:3134:C:H2'   | 1:AS:3135:A:C8     | 2.37                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:BG:36:ARG:HA    | 14:BG:39:ARG:HD3   | 1.83                     | 0.60              |
| 23:BP:101:VAL:HG11 | 23:BP:107:LYS:HZ2  | 1.65                     | 0.60              |
| 59:CZ:130:SER:OG   | 59:CZ:132:GLU:OE1  | 2.19                     | 0.60              |
| 1:1:1774:G:O2'     | 1:1:1776:G:OP2     | 2.20                     | 0.60              |
| 8:n:170:ARG:HB3    | 8:n:172:HIS:CE1    | 2.36                     | 0.60              |
| 47:C:48:ILE:HD12   | 47:C:149:MET:HE3   | 1.84                     | 0.60              |
| 80:BE:193:ASP:OD2  | 80:BE:198:LYS:HE3  | 2.02                     | 0.60              |
| 45:CL:122:THR:OG1  | 50:CQ:125:ARG:HG3  | 2.02                     | 0.60              |
| 52:CS:95:ASN:OD1   | 52:CS:107:LYS:NZ   | 2.34                     | 0.60              |
| 54:CU:32:ALA:HA    | 54:CU:35:ARG:HG3   | 1.84                     | 0.60              |
| 54:CU:163:ASP:O    | 54:CU:167:GLN:HG2  | 2.01                     | 0.60              |
| 79:DT:103:ARG:HE   | 79:DT:105:VAL:CG2  | 2.13                     | 0.60              |
| 1:1:1268:C:H3'     | 1:1:1269:A:H8      | 1.66                     | 0.60              |
| 4:j:247:ARG:HB3    | 46:B:997:U:H4'     | 1.84                     | 0.60              |
| 10:p:152:VAL:O     | 10:p:178:TYR:HA    | 2.02                     | 0.60              |
| 27:9:51:ARG:HG2    | 27:9:52:GLN:N      | 2.15                     | 0.60              |
| 45:i:50:LYS:O      | 45:i:52:LYS:N      | 2.34                     | 0.60              |
| 46:B:563:C:O3'     | 70:Z:66:SER:OG     | 2.19                     | 0.60              |
| 46:B:1400:U:H5''   | 64:T:3:ARG:HE      | 1.67                     | 0.60              |
| 1:AS:85:G:O2'      | 1:AS:97:G:O6       | 2.16                     | 0.60              |
| 1:AS:359:U:OP1     | 38:CE:11:ARG:NH1   | 2.35                     | 0.60              |
| 1:AS:563:U:H2'     | 1:AS:564:G:C8      | 2.37                     | 0.60              |
| 1:AS:820:C:OP1     | 4:AW:21:ARG:NE     | 2.35                     | 0.60              |
| 1:AS:1791:U:H2'    | 4:AW:50:HIS:CD2    | 2.37                     | 0.60              |
| 7:AZ:95:TRP:CD1    | 7:AZ:158:ARG:HA    | 2.36                     | 0.60              |
| 14:BG:57:VAL:HG23  | 14:BG:149:VAL:HG13 | 1.84                     | 0.60              |
| 39:CF:28:ASN:ND2   | 39:CF:42:LYS:HD2   | 2.15                     | 0.60              |
| 46:CM:52:U:H2'     | 46:CM:53:G:H8      | 1.66                     | 0.60              |
| 52:CS:158:GLN:HG2  | 75:DP:66:LEU:HD11  | 1.84                     | 0.60              |
| 52:CS:172:ILE:O    | 52:CS:176:THR:HG23 | 2.01                     | 0.60              |
| 20:z:23:TRP:HB3    | 20:z:51:VAL:HG12   | 1.83                     | 0.60              |
| 46:B:1064:U:H2'    | 46:B:1065:U:C6     | 2.36                     | 0.60              |
| 1:AS:640:U:OP1     | 29:BV:22:ILE:HG23  | 2.02                     | 0.60              |
| 57:CX:58:GLN:HB3   | 57:CX:65:TYR:HB2   | 1.83                     | 0.60              |
| 57:CX:76:LEU:O     | 57:CX:80:LEU:HB2   | 2.01                     | 0.60              |
| 1:1:422:A:C2       | 1:1:2341:A:H4'     | 2.36                     | 0.60              |
| 1:1:638:U:H2'      | 1:1:639:C:C6       | 2.37                     | 0.60              |
| 6:l:60:GLN:O       | 38:AK:52:LYS:NZ    | 2.28                     | 0.60              |
| 45:i:69:PHE:HE1    | 62:R:127:ARG:HD3   | 1.66                     | 0.60              |
| 46:B:213:A:C2'     | 46:B:214:U:H5'     | 2.32                     | 0.60              |
| 59:O:62:LEU:HD11   | 59:O:90:LYS:HD3    | 1.84                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:R:1:MET:CB      | 65:U:18:LEU:H      | 2.15                     | 0.60              |
| 1:AS:1642:G:O2'    | 1:AS:1804:G:N2     | 2.31                     | 0.60              |
| 1:AS:2345:A:H2'    | 1:AS:2346:A:C8     | 2.36                     | 0.60              |
| 1:AS:2500:G:O6     | 4:AW:72:ARG:NH2    | 2.35                     | 0.60              |
| 20:BM:134:HIS:HE1  | 20:BM:136:ARG:HE   | 1.49                     | 0.60              |
| 47:CN:33:ASN:ND2   | 47:CN:148:ASP:O    | 2.34                     | 0.60              |
| 48:CO:49:ASN:O     | 48:CO:55:LYS:NZ    | 2.31                     | 0.60              |
| 48:CO:81:TYR:CB    | 48:CO:109:LYS:HD3  | 2.32                     | 0.60              |
| 54:CU:150:LEU:HB2  | 54:CU:181:ILE:HG12 | 1.84                     | 0.60              |
| 79:DT:107:HIS:HE1  | 79:DT:129:ASP:HB2  | 1.66                     | 0.60              |
| 14:t:49:ARG:HD3    | 36:AI:115:LYS:HA   | 1.83                     | 0.60              |
| 16:v:143:ARG:O     | 16:v:149:ASN:ND2   | 2.35                     | 0.60              |
| 46:B:29:U:H2'      | 46:B:30:G:H8       | 1.67                     | 0.60              |
| 46:B:784:U:H2'     | 46:B:785:G:C8      | 2.36                     | 0.60              |
| 46:B:1237:C:O2'    | 78:h:184:GLY:N     | 2.35                     | 0.60              |
| 46:B:1265:C:H2'    | 46:B:1266:G:H8     | 1.67                     | 0.60              |
| 51:G:192:VAL:HG23  | 51:G:244:GLY:HA3   | 1.83                     | 0.60              |
| 1:AS:2533:G:H21    | 28:BU:135:HIS:HB2  | 1.65                     | 0.60              |
| 1:AS:2869:A:H2'    | 1:AS:2871:C:H5''   | 1.84                     | 0.60              |
| 14:BG:127:ASP:HA   | 36:CC:114:ARG:HH22 | 1.66                     | 0.60              |
| 46:CM:230:U:H5'    | 46:CM:231:C:C6     | 2.36                     | 0.60              |
| 46:CM:636:C:OP2    | 69:DJ:32:LYS:NZ    | 2.27                     | 0.60              |
| 46:CM:916:C:H4'    | 48:CO:115:ARG:O    | 2.02                     | 0.60              |
| 46:CM:1335:U:H2'   | 46:CM:1336:G:C8    | 2.37                     | 0.60              |
| 48:CO:30:PHE:HB2   | 48:CO:96:LEU:HD13  | 1.84                     | 0.60              |
| 48:CO:43:VAL:HG23  | 48:CO:44:GLY:H     | 1.66                     | 0.60              |
| 79:DT:40:LYS:NZ    | 79:DT:66:SER:O     | 2.35                     | 0.60              |
| 79:DT:90:LEU:HB2   | 79:DT:104:PHE:HB2  | 1.84                     | 0.60              |
| 79:DT:201:LEU:HD23 | 79:DT:201:LEU:N    | 2.12                     | 0.60              |
| 1:1:2191:A:H2'     | 1:1:2192:A:H8      | 1.65                     | 0.59              |
| 1:1:3042:A:OP1     | 20:z:62:ARG:NH1    | 2.35                     | 0.59              |
| 1:1:3046:G:H4'     | 32:AE:61:ARG:HD2   | 1.84                     | 0.59              |
| 1:1:3156:A:N6      | 11:q:58:HIS:O      | 2.35                     | 0.59              |
| 4:j:147:ARG:HG2    | 4:j:157:ILE:HG12   | 1.84                     | 0.59              |
| 16:v:27:CYS:HB2    | 16:v:122:ASN:ND2   | 2.17                     | 0.59              |
| 46:B:880:G:H22     | 46:B:902:U:H3      | 1.50                     | 0.59              |
| 46:B:1160:U:H2'    | 46:B:1161:G:H8     | 1.67                     | 0.59              |
| 1:AS:1611:U:H2'    | 1:AS:1612:U:C6     | 2.37                     | 0.59              |
| 1:AS:1762:G:N7     | 20:BM:46:LYS:HE2   | 2.17                     | 0.59              |
| 2:AT:4:U:H2'       | 2:AT:5:G:H8        | 1.67                     | 0.59              |
| 16:BI:46:ASP:OD2   | 16:BI:50:ARG:NH2   | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:CB:101:VAL:O    | 35:CB:105:LEU:HG   | 2.02                     | 0.59              |
| 37:CD:40:ARG:O     | 37:CD:44:LYS:HG3   | 2.02                     | 0.59              |
| 46:CM:1064:U:H2'   | 46:CM:1065:U:C6    | 2.37                     | 0.59              |
| 46:CM:1475:U:OP1   | 50:CQ:10:LYS:NZ    | 2.22                     | 0.59              |
| 46:CM:1615:U:H2'   | 46:CM:1616:G:C8    | 2.37                     | 0.59              |
| 1:1:2852:U:H5''    | 5:k:236:LYS:HG2    | 1.83                     | 0.59              |
| 15:u:116:LEU:HD11  | 17:w:194:LYS:HD2   | 1.85                     | 0.59              |
| 46:B:932:U:H2'     | 46:B:933:A:H8      | 1.67                     | 0.59              |
| 46:B:1669:U:HO2'   | 46:B:1670:U:H6     | 1.50                     | 0.59              |
| 48:D:62:LYS:NZ     | 48:D:90:GLU:HA     | 2.17                     | 0.59              |
| 83:AS:3401:3K5:H13 | 83:AS:3401:3K5:H7  | 1.85                     | 0.59              |
| 11:BD:23:ARG:NH2   | 11:BD:39:LYS:O     | 2.35                     | 0.59              |
| 45:CL:55:LYS:HE2   | 45:CL:55:LYS:HA    | 1.83                     | 0.59              |
| 47:CN:198:MET:HB3  | 64:DE:85:VAL:HG21  | 1.83                     | 0.59              |
| 52:CS:27:THR:OG1   | 63:DD:27:LEU:HD12  | 2.02                     | 0.59              |
| 72:DM:36:ALA:HB1   | 72:DM:38:HIS:CD2   | 2.37                     | 0.59              |
| 79:DT:82:LEU:HD13  | 79:DT:123:ILE:HG21 | 1.84                     | 0.59              |
| 79:DT:159:PRO:HD2  | 79:DT:201:LEU:HD12 | 1.83                     | 0.59              |
| 1:1:164:U:H2'      | 1:1:165:C:C6       | 2.38                     | 0.59              |
| 1:1:1524:G:O2'     | 1:1:1584:A:N3      | 2.31                     | 0.59              |
| 43:AP:61:LYS:NZ    | 43:AP:63:LYS:O     | 2.35                     | 0.59              |
| 45:i:71:LYS:C      | 45:i:73:VAL:H      | 2.09                     | 0.59              |
| 46:B:338:U:H2'     | 46:B:339:A:H8      | 1.68                     | 0.59              |
| 46:B:470:U:H5''    | 56:L:11:THR:HG23   | 1.84                     | 0.59              |
| 46:B:1486:G:OP2    | 66:V:73:VAL:HG12   | 2.02                     | 0.59              |
| 62:R:77:LYS:HD2    | 62:R:102:PHE:CE1   | 2.37                     | 0.59              |
| 63:S:40:PRO:HG3    | 63:S:77:VAL:HG21   | 1.82                     | 0.59              |
| 1:AS:449:U:H2'     | 1:AS:450:G:C8      | 2.36                     | 0.59              |
| 1:AS:2919:G:OP1    | 1:AS:2954:A:N6     | 2.28                     | 0.59              |
| 1:AS:2961:U:O2'    | 5:AX:232:ARG:NH1   | 2.36                     | 0.59              |
| 1:AS:3039:C:H3'    | 20:BM:62:ARG:HH22  | 1.68                     | 0.59              |
| 4:AW:242:ARG:NH2   | 4:AW:243:THR:O     | 2.35                     | 0.59              |
| 8:BA:70:VAL:HG13   | 8:BA:160:ALA:HB2   | 1.84                     | 0.59              |
| 10:BC:192:HIS:O    | 10:BC:193:LYS:HD3  | 2.03                     | 0.59              |
| 46:CM:1220:C:H5    | 78:DS:180:ARG:HE   | 1.48                     | 0.59              |
| 46:CM:1672:G:O2'   | 46:CM:1673:U:H5'   | 2.01                     | 0.59              |
| 62:DC:91:GLY:H     | 62:DC:107:ILE:HB   | 1.67                     | 0.59              |
| 1:1:1104:U:H2'     | 1:1:1105:U:C6      | 2.37                     | 0.59              |
| 1:1:2625:C:OP1     | 43:AP:89:LYS:HB2   | 2.02                     | 0.59              |
| 7:m:164:LYS:NZ     | 7:m:168:ASP:OD1    | 2.35                     | 0.59              |
| 45:i:68:ASN:O      | 45:i:69:PHE:HB2    | 2.02                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:B:480:U:H2'     | 46:B:481:A:C8     | 2.37                     | 0.59              |
| 46:B:1026:G:H2'    | 46:B:1027:G:H8    | 1.65                     | 0.59              |
| 46:B:1469:A:H2'    | 46:B:1470:G:C8    | 2.37                     | 0.59              |
| 46:B:1552:C:H5''   | 65:U:41:ARG:HG2   | 1.85                     | 0.59              |
| 1:AS:941:C:H2'     | 1:AS:942:U:C6     | 2.38                     | 0.59              |
| 1:AS:1173:G:N7     | 34:CA:20:LYS:NZ   | 2.43                     | 0.59              |
| 10:BC:181:VAL:HG22 | 10:BC:182:LYS:H   | 1.67                     | 0.59              |
| 13:BF:90:GLN:HG3   | 13:BF:170:GLU:HB2 | 1.84                     | 0.59              |
| 46:CM:876:A:H2'    | 46:CM:877:G:C8    | 2.37                     | 0.59              |
| 46:CM:1301:G:HO2'  | 46:CM:1387:A:HO2' | 1.50                     | 0.59              |
| 50:CQ:59:VAL:HG12  | 50:CQ:60:LEU:HD12 | 1.84                     | 0.59              |
| 52:CS:99:MET:O     | 52:CS:103:ASN:HB2 | 2.02                     | 0.59              |
| 79:DT:9:LEU:HB2    | 79:DT:310:TRP:CZ3 | 2.37                     | 0.59              |
| 79:DT:16:HIS:CE1   | 79:DT:37:SER:CB   | 2.85                     | 0.59              |
| 81:P0:23:LYS:HA    | 81:P0:23:LYS:HE3  | 1.84                     | 0.59              |
| 1:1:1456:A:H2'     | 1:1:1457:A:C8     | 2.37                     | 0.59              |
| 1:1:2244:U:H2'     | 1:1:2245:C:C6     | 2.37                     | 0.59              |
| 1:1:2384:C:H2'     | 1:1:2385:C:C6     | 2.38                     | 0.59              |
| 27:9:112:ASP:O     | 27:9:116:LYS:HG2  | 2.03                     | 0.59              |
| 46:B:58:U:O2'      | 46:B:449:G:N3     | 2.33                     | 0.59              |
| 46:B:217:A:N7      | 46:B:218:A:C8     | 2.70                     | 0.59              |
| 46:B:1245:U:H2'    | 46:B:1246:G:H8    | 1.66                     | 0.59              |
| 62:R:1:MET:HB3     | 65:U:17:LEU:HA    | 1.85                     | 0.59              |
| 68:X:58:TYR:OH     | 69:Y:20:THR:HA    | 2.02                     | 0.59              |
| 14:BG:194:GLU:O    | 14:BG:198:GLU:HG3 | 2.02                     | 0.59              |
| 23:BP:30:GLN:HE21  | 23:BP:58:ALA:HB1  | 1.67                     | 0.59              |
| 32:BY:45:THR:HG22  | 32:BY:47:ASP:H    | 1.67                     | 0.59              |
| 57:CX:70:ASP:OD1   | 57:CX:71:GLU:N    | 2.36                     | 0.59              |
| 59:CZ:116:VAL:O    | 59:CZ:118:ALA:N   | 2.35                     | 0.59              |
| 1:1:2138:G:H2'     | 1:1:2139:G:H8     | 1.66                     | 0.59              |
| 46:B:265:U:H2'     | 46:B:266:C:H6     | 1.67                     | 0.59              |
| 47:C:36:TYR:OH     | 47:C:56:LYS:NZ    | 2.34                     | 0.59              |
| 1:AS:248:U:H2'     | 1:AS:249:G:H4'    | 1.83                     | 0.59              |
| 1:AS:2171:U:O4     | 1:AS:2221:A:N6    | 2.35                     | 0.59              |
| 45:CL:165:LEU:HD12 | 45:CL:165:LEU:O   | 2.02                     | 0.59              |
| 46:CM:218:A:H5''   | 46:CM:218:A:H8    | 1.67                     | 0.59              |
| 52:CS:213:LYS:O    | 52:CS:217:LEU:HG  | 2.03                     | 0.59              |
| 1:1:1080:A:H2'     | 1:1:1081:A:C8     | 2.38                     | 0.59              |
| 1:1:1301:U:C2      | 5:k:257:PRO:HG3   | 2.38                     | 0.59              |
| 45:i:115:LEU:O     | 45:i:118:GLU:N    | 2.35                     | 0.59              |
| 46:B:822:G:H3'     | 46:B:823:G:C5'    | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:F:143:LEU:O     | 50:F:145:ALA:N     | 2.33                     | 0.59              |
| 51:G:63:ALA:O      | 51:G:67:GLN:HG2    | 2.03                     | 0.59              |
| 63:S:131:ARG:HG3   | 63:S:137:PHE:HE1   | 1.67                     | 0.59              |
| 3:AU:63:G:H1       | 3:AU:97:A:H61      | 1.50                     | 0.59              |
| 4:AW:27:ALA:O      | 4:AW:128:ARG:NH2   | 2.35                     | 0.59              |
| 26:BS:88:ILE:HD11  | 26:BS:114:ILE:HD13 | 1.84                     | 0.59              |
| 27:BT:58:VAL:HA    | 27:BT:104:VAL:HG12 | 1.84                     | 0.59              |
| 52:CS:42:LEU:HB3   | 52:CS:46:TRP:HD1   | 1.66                     | 0.59              |
| 52:CS:62:ILE:HD12  | 52:CS:89:ILE:HD13  | 1.84                     | 0.59              |
| 52:CS:142:ALA:O    | 52:CS:167:ARG:HG2  | 2.02                     | 0.59              |
| 1:1:172:C:O2'      | 1:1:173:C:OP1      | 2.21                     | 0.59              |
| 10:p:252:LYS:HE3   | 10:p:256:ALA:HB2   | 1.84                     | 0.59              |
| 23:5:15:PHE:HB2    | 23:5:66:VAL:HB     | 1.84                     | 0.59              |
| 46:B:518:A:H2'     | 46:B:519:A:C8      | 2.37                     | 0.59              |
| 46:B:881:U:H5'     | 48:D:23:PRO:HG2    | 1.83                     | 0.59              |
| 46:B:886:G:H2'     | 46:B:887:G:C8      | 2.38                     | 0.59              |
| 46:B:1659:G:H2'    | 46:B:1660:G:C8     | 2.37                     | 0.59              |
| 64:T:96:THR:HG23   | 64:T:98:GLY:H      | 1.67                     | 0.59              |
| 66:V:107:ALA:O     | 66:V:111:ILE:HG12  | 2.02                     | 0.59              |
| 1:AS:1007:A:H2'    | 1:AS:1008:A:C8     | 2.38                     | 0.59              |
| 1:AS:1713:U:H2'    | 1:AS:1714:G:H8     | 1.66                     | 0.59              |
| 1:AS:2632:G:OP1    | 1:AS:2722:U:O2'    | 2.19                     | 0.59              |
| 10:BC:158:VAL:HG21 | 10:BC:164:VAL:HG21 | 1.83                     | 0.59              |
| 23:BP:19:VAL:HG11  | 23:BP:23:VAL:HG23  | 1.85                     | 0.59              |
| 46:CM:1266:G:O3'   | 67:DH:75:SER:OG    | 2.17                     | 0.59              |
| 54:CU:55:ALA:HA    | 54:CU:87:VAL:HG23  | 1.85                     | 0.59              |
| 54:CU:158:VAL:O    | 54:CU:160:TYR:N    | 2.35                     | 0.59              |
| 75:DP:40:ILE:HG23  | 75:DP:62:GLU:HG3   | 1.85                     | 0.59              |
| 79:DT:12:THR:HG23  | 79:DT:53:ASN:ND2   | 2.18                     | 0.59              |
| 79:DT:313:MET:HG3  | 79:DT:314:THR:N    | 2.10                     | 0.59              |
| 1:1:1642:G:H1'     | 1:1:1805:A:N6      | 2.16                     | 0.59              |
| 46:B:63:G:O2'      | 46:B:168:U:OP1     | 2.19                     | 0.59              |
| 46:B:759:A:N6      | 46:B:770:C:H42     | 2.01                     | 0.59              |
| 46:B:821:U:H2'     | 46:B:822:G:H8      | 1.67                     | 0.59              |
| 1:AS:479:C:H2'     | 1:AS:480:G:C8      | 2.37                     | 0.59              |
| 1:AS:1662:G:H2'    | 1:AS:1663:A:C8     | 2.36                     | 0.59              |
| 5:AX:292:ALA:HB1   | 5:AX:295:ALA:HB3   | 1.84                     | 0.59              |
| 46:CM:487:C:O2     | 46:CM:496:G:N2     | 2.35                     | 0.59              |
| 48:CO:114:VAL:HG22 | 48:CO:142:PHE:HZ   | 1.68                     | 0.59              |
| 48:CO:159:SER:O    | 48:CO:163:GLU:HG3  | 2.03                     | 0.59              |
| 50:CQ:19:TYR:HE1   | 50:CQ:38:VAL:HG13  | 1.68                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:CR:148:ARG:NH2 | 53:CT:201:GLN:OE1  | 2.36                     | 0.59              |
| 79:DT:126:ALA:HB2 | 79:DT:155:VAL:CG1  | 2.25                     | 0.59              |
| 1:1:730:A:H4'     | 1:1:730:A:OP1      | 2.03                     | 0.59              |
| 4:j:204:MET:SD    | 4:j:209:HIS:HB2    | 2.43                     | 0.59              |
| 13:s:109:HIS:HD2  | 13:s:123:TYR:H     | 1.50                     | 0.59              |
| 31:AD:11:ASN:HD22 | 31:AD:11:ASN:H     | 1.50                     | 0.59              |
| 46:B:972:G:N2     | 46:B:998:A:OP1     | 2.34                     | 0.59              |
| 59:O:96:LEU:HD12  | 59:O:100:TRP:HZ3   | 1.67                     | 0.59              |
| 63:S:27:LEU:HD11  | 63:S:29:LYS:NZ     | 2.18                     | 0.59              |
| 14:BG:4:SER:OG    | 14:BG:5:LYS:NZ     | 2.30                     | 0.59              |
| 17:BJ:122:PRO:HA  | 17:BJ:125:LEU:HD12 | 1.84                     | 0.59              |
| 21:BN:96:ASP:OD1  | 21:BN:97:VAL:N     | 2.36                     | 0.59              |
| 28:BU:121:LYS:O   | 28:BU:127:ASN:ND2  | 2.29                     | 0.59              |
| 54:CU:83:ASP:OD1  | 54:CU:84:ARG:HG3   | 2.03                     | 0.59              |
| 64:DE:89:SER:HB3  | 64:DE:92:ASP:HB2   | 1.85                     | 0.59              |
| 1:1:1230:G:H2'    | 1:1:1231:U:C6      | 2.38                     | 0.58              |
| 1:1:1552:C:H5''   | 1:1:2147:G:N2      | 2.18                     | 0.58              |
| 1:1:2431:U:C6     | 1:1:2439:A:H5''    | 2.38                     | 0.58              |
| 1:1:2729:U:H4'    | 22:2:7:TYR:HB3     | 1.85                     | 0.58              |
| 46:B:1145:A:H2'   | 46:B:1146:C:C6     | 2.38                     | 0.58              |
| 1:AS:1035:U:H2'   | 1:AS:1036:A:C8     | 2.38                     | 0.58              |
| 1:AS:3021:A:C5    | 5:AX:75:ALA:HB2    | 2.38                     | 0.58              |
| 45:CL:95:GLY:C    | 45:CL:96:LYS:HD3   | 2.28                     | 0.58              |
| 46:CM:638:U:C4    | 54:CU:114:LEU:HD21 | 2.37                     | 0.58              |
| 46:CM:694:C:H3'   | 46:CM:695:C:C5'    | 2.25                     | 0.58              |
| 46:CM:723:G:C4    | 46:CM:724:G:H1'    | 2.38                     | 0.58              |
| 46:CM:1221:A:C4   | 78:DS:180:ARG:NH2  | 2.70                     | 0.58              |
| 48:CO:58:ALA:HB1  | 48:CO:91:VAL:HG11  | 1.85                     | 0.58              |
| 52:CS:27:THR:N    | 63:DD:26:GLY:O     | 2.33                     | 0.58              |
| 56:CW:101:PRO:O   | 56:CW:105:LEU:HD12 | 2.02                     | 0.58              |
| 81:P0:38:MET:HA   | 81:P0:41:ILE:HD12  | 1.85                     | 0.58              |
| 1:1:833:A:OP2     | 44:AQ:4:ARG:NH1    | 2.36                     | 0.58              |
| 1:1:1580:U:H2'    | 1:1:1581:C:H6      | 1.68                     | 0.58              |
| 83:1:3401:3K5:H13 | 43:AP:57:ILE:HG23  | 1.84                     | 0.58              |
| 7:m:231:ILE:HG21  | 7:m:239:ILE:HD11   | 1.86                     | 0.58              |
| 17:w:116:LYS:O    | 17:w:118:ARG:NH1   | 2.36                     | 0.58              |
| 28:AA:85:TYR:OH   | 35:AH:97:GLU:OE2   | 2.21                     | 0.58              |
| 53:I:161:GLU:HB3  | 53:I:170:THR:HG22  | 1.84                     | 0.58              |
| 1:AS:155:A:OP2    | 37:CD:24:LYS:NZ    | 2.35                     | 0.58              |
| 1:AS:1208:A:O3'   | 21:BN:92:LYS:NZ    | 2.36                     | 0.58              |
| 1:AS:2650:A:OP1   | 45:CL:57:PRO:HD2   | 2.02                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:2876:U:H2'    | 1:AS:2877:U:H6     | 1.67                     | 0.58              |
| 5:AX:260:VAL:HG11  | 5:AX:266:ARG:HH11  | 1.68                     | 0.58              |
| 25:BR:86:SER:OG    | 25:BR:88:GLU:OE1   | 2.17                     | 0.58              |
| 25:BR:103:ALA:HA   | 25:BR:106:ASP:HB2  | 1.83                     | 0.58              |
| 26:BS:73:MET:HE1   | 26:BS:141:TYR:HE2  | 1.68                     | 0.58              |
| 46:CM:1003:U:OP1   | 60:DA:107:LYS:NZ   | 2.36                     | 0.58              |
| 49:CP:39:LEU:HD12  | 49:CP:235:LEU:HD23 | 1.85                     | 0.58              |
| 52:CS:42:LEU:HD12  | 52:CS:69:PHE:O     | 2.02                     | 0.58              |
| 62:DC:52:LYS:HB3   | 62:DC:80:LEU:HD11  | 1.85                     | 0.58              |
| 76:DQ:19:ARG:HD2   | 76:DQ:32:ARG:HD3   | 1.83                     | 0.58              |
| 79:DT:132:VAL:O    | 79:DT:145:LEU:HB3  | 2.03                     | 0.58              |
| 2:3:4:U:H2'        | 2:3:5:G:H8         | 1.68                     | 0.58              |
| 53:I:21:GLU:OE2    | 53:I:28:TYR:OH     | 2.19                     | 0.58              |
| 65:U:87:ASN:HB2    | 65:U:99:HIS:CE1    | 2.38                     | 0.58              |
| 70:Z:37:ALA:HA     | 70:Z:41:SER:HB3    | 1.85                     | 0.58              |
| 70:Z:109:ARG:HB3   | 70:Z:112:LYS:HG3   | 1.85                     | 0.58              |
| 78:h:157:GLU:CG    | 78:h:159:LEU:HG    | 2.33                     | 0.58              |
| 5:AX:260:VAL:HG11  | 5:AX:266:ARG:NH1   | 2.18                     | 0.58              |
| 9:BB:71:ASN:O      | 22:BO:143:THR:OG1  | 2.20                     | 0.58              |
| 28:BU:3:LYS:HB3    | 28:BU:6:LYS:NZ     | 2.18                     | 0.58              |
| 28:BU:134:LEU:HD23 | 28:BU:136:PHE:HE1  | 1.68                     | 0.58              |
| 46:CM:302:U:H2'    | 46:CM:303:C:C6     | 2.38                     | 0.58              |
| 52:CS:214:LYS:O    | 52:CS:218:GLU:HG3  | 2.03                     | 0.58              |
| 54:CU:25:GLU:O     | 54:CU:31:LYS:HD2   | 2.02                     | 0.58              |
| 65:DF:134:ARG:HB2  | 65:DF:136:GLN:NE2  | 2.18                     | 0.58              |
| 1:1:1468:U:H5''    | 20:z:24:LEU:HD12   | 1.84                     | 0.58              |
| 14:t:49:ARG:HG2    | 36:AI:116:PHE:O    | 2.03                     | 0.58              |
| 46:B:309:U:OP2     | 70:Z:20:ARG:HD3    | 2.03                     | 0.58              |
| 46:B:480:U:H2'     | 46:B:481:A:H8      | 1.67                     | 0.58              |
| 46:B:915:A:H2'     | 48:D:114:VAL:HG11  | 1.85                     | 0.58              |
| 46:B:965:G:H4'     | 46:B:1763:A:H4'    | 1.84                     | 0.58              |
| 46:B:1779:G:OP1    | 73:c:8:ASN:ND2     | 2.35                     | 0.58              |
| 55:K:113:TYR:OH    | 55:K:156:ALA:O     | 2.14                     | 0.58              |
| 1:AS:1580:U:H2'    | 1:AS:1581:C:H6     | 1.67                     | 0.58              |
| 47:CN:79:ARG:NH2   | 47:CN:165:LYS:HG2  | 2.18                     | 0.58              |
| 48:CO:22:ASP:C     | 48:CO:24:PHE:H     | 2.10                     | 0.58              |
| 48:CO:66:PHE:CD2   | 61:DB:29:SER:HB2   | 2.38                     | 0.58              |
| 52:CS:216:GLU:O    | 52:CS:220:VAL:HG22 | 2.03                     | 0.58              |
| 64:DE:99:GLN:OE1   | 64:DE:120:GLN:NE2  | 2.34                     | 0.58              |
| 79:DT:249:LEU:O    | 79:DT:260:PHE:HD2  | 1.87                     | 0.58              |
| 4:j:242:ARG:NH2    | 4:j:243:THR:O      | 2.37                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:6:42:THR:HG21  | 24:6:50:PRO:HG3    | 1.85                     | 0.58              |
| 42:AO:18:ARG:NH1  | 46:B:1110:A:OP1    | 2.36                     | 0.58              |
| 46:B:330:U:P      | 55:K:56:ARG:HH22   | 2.27                     | 0.58              |
| 46:B:477:C:OP1    | 56:L:121:SER:OG    | 2.17                     | 0.58              |
| 55:K:56:ARG:NH1   | 55:K:180:GLY:O     | 2.36                     | 0.58              |
| 1:AS:2920:C:H5''  | 5:AX:243:HIS:HB3   | 1.85                     | 0.58              |
| 23:BP:85:LYS:HE3  | 23:BP:89:LYS:HE3   | 1.86                     | 0.58              |
| 28:BU:48:ARG:HG3  | 28:BU:69:LYS:HB3   | 1.84                     | 0.58              |
| 46:CM:390:G:OP1   | 55:CV:24:LYS:NZ    | 2.31                     | 0.58              |
| 51:CR:152:PRO:HD2 | 53:CT:211:LEU:HD22 | 1.86                     | 0.58              |
| 54:CU:52:LYS:HE2  | 54:CU:84:ARG:NH1   | 2.19                     | 0.58              |
| 1:1:2638:C:OP2    | 1:1:2659:G:N1      | 2.35                     | 0.58              |
| 3:4:69:U:H3       | 3:4:89:A:H61       | 1.51                     | 0.58              |
| 14:t:133:SER:HA   | 14:BG:129:LYS:HE3  | 1.84                     | 0.58              |
| 46:B:1276:G:H22   | 46:B:1309:G:N2     | 2.01                     | 0.58              |
| 46:B:1399:U:OP2   | 64:T:3:ARG:NH2     | 2.37                     | 0.58              |
| 1:AS:1106:U:H2'   | 1:AS:1107:U:C6     | 2.38                     | 0.58              |
| 1:AS:1225:G:H2'   | 1:AS:1226:G:C8     | 2.38                     | 0.58              |
| 1:AS:1683:U:H1'   | 23:BP:78:TYR:CD2   | 2.39                     | 0.58              |
| 1:AS:2943:A:H2'   | 1:AS:2943:A:N3     | 2.18                     | 0.58              |
| 6:AY:303:ALA:HB2  | 19:BL:39:ARG:HH12  | 1.67                     | 0.58              |
| 13:BF:77:GLU:OE2  | 13:BF:167:TYR:OH   | 2.18                     | 0.58              |
| 46:CM:788:A:C8    | 69:DJ:107:SER:HA   | 2.38                     | 0.58              |
| 46:CM:875:C:H2'   | 46:CM:876:A:H8     | 1.67                     | 0.58              |
| 46:CM:1543:A:P    | 62:DC:44:ARG:HD3   | 2.44                     | 0.58              |
| 54:CU:27:GLN:HB3  | 54:CU:29:ASP:OD1   | 2.03                     | 0.58              |
| 78:DS:178:LYS:NZ  | 78:DS:179:ASP:OD2  | 2.35                     | 0.58              |
| 1:1:2528:U:O4'    | 10:p:39:GLN:NE2    | 2.37                     | 0.58              |
| 5:k:106:TRP:HB2   | 5:k:133:TYR:CE2    | 2.39                     | 0.58              |
| 12:r:43:VAL:HG21  | 12:r:197:VAL:HG13  | 1.84                     | 0.58              |
| 13:s:32:ARG:NH1   | 13:s:123:TYR:OH    | 2.37                     | 0.58              |
| 23:5:19:VAL:O     | 23:5:21:ALA:N      | 2.36                     | 0.58              |
| 50:F:72:SER:O     | 50:F:76:LYS:HD2    | 2.04                     | 0.58              |
| 1:AS:290:G:H1'    | 16:BI:93:LYS:HD2   | 1.86                     | 0.58              |
| 1:AS:2492:U:OP2   | 1:AS:2558:G:N2     | 2.36                     | 0.58              |
| 1:AS:2634:G:H2'   | 1:AS:2635:A:H8     | 1.67                     | 0.58              |
| 1:AS:2655:U:H2'   | 1:AS:2656:C:H6     | 1.64                     | 0.58              |
| 9:BB:143:ARG:HG3  | 9:BB:183:ILE:HD13  | 1.86                     | 0.58              |
| 46:CM:515:U:H2'   | 46:CM:516:A:C8     | 2.39                     | 0.58              |
| 46:CM:1127:A:H5'' | 73:DN:2:PRO:HB3    | 1.85                     | 0.58              |
| 52:CS:210:ALA:HA  | 52:CS:213:LYS:HB2  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:527:G:H2'     | 1:1:528:A:C8       | 2.38                     | 0.58              |
| 7:m:48:LYS:HG2    | 7:m:145:PHE:HE2    | 1.68                     | 0.58              |
| 19:y:94:LEU:HD22  | 29:AB:119:PRO:HG3  | 1.84                     | 0.58              |
| 46:B:558:U:H2'    | 46:B:559:G:H8      | 1.69                     | 0.58              |
| 48:D:58:ALA:O     | 48:D:62:LYS:HG3    | 2.04                     | 0.58              |
| 67:W:20:LYS:HD3   | 67:W:93:GLN:HG2    | 1.83                     | 0.58              |
| 67:W:26:THR:OG1   | 67:W:112:ASP:OD1   | 2.20                     | 0.58              |
| 75:e:14:LYS:HB3   | 75:e:29:ARG:HB3    | 1.86                     | 0.58              |
| 1:AS:629:A:C2     | 34:CA:91:PRO:HG2   | 2.38                     | 0.58              |
| 1:AS:2888:U:H5    | 1:AS:2907:U:HO2'   | 1.50                     | 0.58              |
| 13:BF:81:GLU:O    | 13:BF:85:LYS:HG3   | 2.04                     | 0.58              |
| 46:CM:483:A:H2'   | 46:CM:484:G:C8     | 2.39                     | 0.58              |
| 55:CV:76:THR:OG1  | 55:CV:105:ASP:HB3  | 2.04                     | 0.58              |
| 57:CX:54:TYR:CE1  | 57:CX:75:PHE:HB2   | 2.38                     | 0.58              |
| 59:CZ:77:ALA:HB3  | 78:DS:156:VAL:HB   | 1.86                     | 0.58              |
| 63:DD:98:GLU:HG3  | 63:DD:101:LYS:HE3  | 1.84                     | 0.58              |
| 1:1:1542:A:N7     | 16:v:71:ARG:NH1    | 2.52                     | 0.58              |
| 1:1:3316:U:H3     | 55:K:110:ARG:NH1   | 2.01                     | 0.58              |
| 5:k:139:THR:OG1   | 5:k:140:ASP:N      | 2.37                     | 0.58              |
| 46:B:1459:U:OP1   | 52:H:183:SER:OG    | 2.20                     | 0.58              |
| 63:S:98:GLU:OE1   | 79:AR:61:SER:N     | 2.37                     | 0.58              |
| 79:AR:96:GLU:HG2  | 79:AR:97:THR:HG23  | 1.86                     | 0.58              |
| 1:AS:1443:G:N7    | 18:BK:25:SER:OG    | 2.35                     | 0.58              |
| 1:AS:2634:G:H2'   | 1:AS:2635:A:C8     | 2.38                     | 0.58              |
| 5:AX:372:THR:HG22 | 5:AX:374:ALA:H     | 1.68                     | 0.58              |
| 14:BG:127:ASP:CG  | 14:BG:130:THR:HG23 | 2.29                     | 0.58              |
| 21:BN:132:THR:O   | 21:BN:141:LYS:NZ   | 2.36                     | 0.58              |
| 58:CY:102:LYS:O   | 70:DK:13:ARG:NH1   | 2.23                     | 0.58              |
| 62:DC:17:PHE:O    | 62:DC:20:VAL:N     | 2.30                     | 0.58              |
| 79:DT:270:GLU:O   | 79:DT:272:LYS:N    | 2.36                     | 0.58              |
| 81:P0:42:ARG:CZ   | 81:P0:51:VAL:HB    | 2.33                     | 0.58              |
| 1:1:544:U:H5'     | 1:1:546:C:H5''     | 1.86                     | 0.58              |
| 1:1:1099:A:N6     | 1:1:1359:A:H1'     | 2.19                     | 0.58              |
| 1:1:1182:G:OP2    | 15:u:36:LYS:NZ     | 2.24                     | 0.58              |
| 1:1:2345:A:H2'    | 1:1:2346:A:C8      | 2.38                     | 0.58              |
| 46:B:52:U:H2'     | 46:B:53:G:C8       | 2.39                     | 0.58              |
| 46:B:515:U:H2'    | 46:B:516:A:C8      | 2.38                     | 0.58              |
| 46:B:1145:A:H2'   | 46:B:1146:C:H6     | 1.68                     | 0.58              |
| 62:R:1:MET:HB2    | 65:U:18:LEU:H      | 1.69                     | 0.58              |
| 1:AS:2876:U:H2'   | 1:AS:2877:U:C6     | 2.39                     | 0.58              |
| 1:AS:3196:U:H2'   | 1:AS:3197:G:H8     | 1.68                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:CL:77:GLN:HG3   | 46:CM:1446:A:H62   | 1.69                     | 0.58              |
| 48:CO:43:VAL:HG12  | 48:CO:73:LEU:HD21  | 1.86                     | 0.58              |
| 61:DB:124:LYS:HG3  | 61:DB:125:GLY:N    | 2.18                     | 0.58              |
| 79:DT:6:VAL:O      | 79:DT:312:VAL:HA   | 2.04                     | 0.58              |
| 1:1:1250:C:H2'     | 1:1:1251:C:H6      | 1.69                     | 0.57              |
| 2:3:7:G:OP1        | 7:m:33:ARG:NH1     | 2.37                     | 0.57              |
| 46:B:1478:A:O2'    | 46:B:1479:A:O4'    | 2.21                     | 0.57              |
| 46:B:1742:A:H2'    | 46:B:1743:A:C8     | 2.39                     | 0.57              |
| 48:D:82:ARG:NH2    | 48:D:191:GLU:OE2   | 2.37                     | 0.57              |
| 66:V:27:LYS:HG2    | 66:V:111:ILE:HD12  | 1.85                     | 0.57              |
| 1:AS:2841:U:O2'    | 1:AS:2845:U:OP1    | 2.21                     | 0.57              |
| 1:AS:3153:A:H2     | 1:AS:3158:G:H4'    | 1.68                     | 0.57              |
| 16:BI:155:VAL:O    | 16:BI:162:ARG:NH2  | 2.26                     | 0.57              |
| 23:BP:20:ALA:H     | 23:BP:62:ASN:CG    | 2.12                     | 0.57              |
| 46:CM:29:U:H2'     | 46:CM:30:G:H8      | 1.69                     | 0.57              |
| 48:CO:24:PHE:CD1   | 48:CO:27:LYS:HE2   | 2.32                     | 0.57              |
| 48:CO:135:LEU:HD13 | 48:CO:137:VAL:HG23 | 1.87                     | 0.57              |
| 50:CQ:128:MET:HE3  | 50:CQ:155:ASP:HB3  | 1.85                     | 0.57              |
| 62:DC:60:LEU:HD21  | 62:DC:94:VAL:HG12  | 1.85                     | 0.57              |
| 1:1:601:U:H4'      | 1:1:602:A:OP1      | 2.01                     | 0.57              |
| 1:1:1842:C:OP1     | 1:1:1845:C:N4      | 2.37                     | 0.57              |
| 1:1:2655:U:H2'     | 1:1:2656:C:H6      | 1.66                     | 0.57              |
| 1:1:2958:U:H2'     | 1:1:2959:A:H8      | 1.69                     | 0.57              |
| 1:1:3225:G:OP2     | 15:u:121:ARG:NH1   | 2.37                     | 0.57              |
| 46:B:738:A:OP1     | 51:G:187:ARG:N     | 2.37                     | 0.57              |
| 46:B:1370:A:OP1    | 67:W:34:GLU:HG3    | 2.03                     | 0.57              |
| 46:B:1719:A:H2'    | 46:B:1720:C:H6     | 1.69                     | 0.57              |
| 62:R:97:TYR:HE1    | 62:R:102:PHE:CE1   | 2.22                     | 0.57              |
| 76:f:19:ARG:HD2    | 76:f:32:ARG:HD3    | 1.85                     | 0.57              |
| 1:AS:627:U:H2'     | 1:AS:628:A:H8      | 1.68                     | 0.57              |
| 10:BC:54:PRO:O     | 10:BC:58:ARG:HG3   | 2.05                     | 0.57              |
| 14:BG:141:VAL:HG21 | 36:CC:118:ILE:HB   | 1.85                     | 0.57              |
| 26:BS:73:MET:HE1   | 26:BS:141:TYR:CE2  | 2.39                     | 0.57              |
| 48:CO:138:PHE:HB3  | 48:CO:213:ARG:HE   | 1.69                     | 0.57              |
| 48:CO:223:PHE:CZ   | 48:CO:228:LEU:HD13 | 2.39                     | 0.57              |
| 58:CY:7:VAL:HG23   | 58:CY:8:GLN:HG2    | 1.86                     | 0.57              |
| 59:CZ:36:LEU:HD21  | 59:CZ:102:GLY:HA3  | 1.86                     | 0.57              |
| 65:DF:63:GLN:O     | 65:DF:67:GLU:HG3   | 2.04                     | 0.57              |
| 66:DG:42:GLY:HA3   | 66:DG:94:VAL:HG21  | 1.87                     | 0.57              |
| 81:P0:34:SER:HB3   | 81:P0:37:GLN:HG3   | 1.86                     | 0.57              |
| 81:P0:44:ALA:O     | 81:P0:45:LEU:HD23  | 2.03                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1124:U:OP1    | 12:r:4:ARG:NH1    | 2.33                     | 0.57              |
| 6:l:157:PHE:CD1   | 6:l:169:VAL:HG11  | 2.39                     | 0.57              |
| 20:z:159:ALA:HA   | 20:z:162:ARG:HH21 | 1.69                     | 0.57              |
| 46:B:17:C:H2'     | 46:B:18:C:C6      | 2.38                     | 0.57              |
| 46:B:511:U:H2'    | 46:B:512:G:C8     | 2.39                     | 0.57              |
| 47:C:88:LYS:HG3   | 47:C:201:LEU:HD11 | 1.86                     | 0.57              |
| 62:R:77:LYS:HD2   | 62:R:102:PHE:CZ   | 2.39                     | 0.57              |
| 63:S:36:THR:HG23  | 63:S:37:LEU:HG    | 1.85                     | 0.57              |
| 1:AS:401:U:H1'    | 1:AS:403:C:C4     | 2.38                     | 0.57              |
| 1:AS:559:C:H2'    | 1:AS:560:C:H6     | 1.70                     | 0.57              |
| 1:AS:1104:U:H2'   | 1:AS:1105:U:C6    | 2.39                     | 0.57              |
| 1:AS:2201:A:H2'   | 1:AS:2202:A:C8    | 2.39                     | 0.57              |
| 3:AU:26:U:H2'     | 3:AU:27:U:C6      | 2.39                     | 0.57              |
| 46:CM:74:U:H1'    | 46:CM:76:A:OP2    | 2.05                     | 0.57              |
| 46:CM:1049:G:O2'  | 48:CO:204:ILE:O   | 2.23                     | 0.57              |
| 70:DK:57:ILE:C    | 77:DR:8:LEU:HD21  | 2.30                     | 0.57              |
| 81:P0:56:ASN:HB3  | 81:P0:60:ARG:HH21 | 1.69                     | 0.57              |
| 1:1:1303:G:C4     | 17:w:61:LYS:HD3   | 2.39                     | 0.57              |
| 1:1:2128:G:O2'    | 1:1:2167:U:OP1    | 2.20                     | 0.57              |
| 46:B:418:A:OP1    | 53:I:96:SER:OG    | 2.17                     | 0.57              |
| 46:B:444:A:OP1    | 51:G:57:ASN:ND2   | 2.37                     | 0.57              |
| 46:B:768:C:H2'    | 46:B:769:U:O4'    | 2.05                     | 0.57              |
| 50:F:143:LEU:HA   | 50:F:180:GLN:HE21 | 1.70                     | 0.57              |
| 1:AS:339:C:OP1    | 1:AS:1376:G:O2'   | 2.15                     | 0.57              |
| 46:CM:267:G:H2'   | 46:CM:268:C:H6    | 1.69                     | 0.57              |
| 52:CS:82:PHE:CZ   | 75:DP:49:ARG:HB2  | 2.39                     | 0.57              |
| 1:1:783:G:H2'     | 1:1:784:C:C6      | 2.39                     | 0.57              |
| 1:1:1580:U:H2'    | 1:1:1581:C:C6     | 2.40                     | 0.57              |
| 46:B:1087:G:OP2   | 70:Z:7:ARG:NH1    | 2.37                     | 0.57              |
| 46:B:1192:C:N3    | 46:B:1442:C:H5    | 2.03                     | 0.57              |
| 46:B:1774:C:OP1   | 61:Q:122:ARG:NH2  | 2.36                     | 0.57              |
| 53:I:64:LYS:NZ    | 53:I:82:SER:OG    | 2.35                     | 0.57              |
| 59:O:47:GLU:HG2   | 59:O:50:LYS:HE2   | 1.87                     | 0.57              |
| 59:O:74:LEU:HA    | 78:h:150:VAL:HG11 | 1.85                     | 0.57              |
| 1:AS:2158:A:H2'   | 1:AS:2159:C:C6    | 2.39                     | 0.57              |
| 26:BS:62:ILE:O    | 26:BS:86:VAL:HG13 | 2.05                     | 0.57              |
| 29:BV:36:GLY:HA3  | 29:BV:40:HIS:CE1  | 2.39                     | 0.57              |
| 45:CL:108:GLY:HA3 | 50:CQ:117:ARG:CG  | 2.34                     | 0.57              |
| 46:CM:482:C:H2'   | 46:CM:483:A:H8    | 1.69                     | 0.57              |
| 46:CM:1070:G:N2   | 46:CM:1073:A:OP2  | 2.33                     | 0.57              |
| 46:CM:1399:U:N3   | 46:CM:1570:A:OP2  | 2.29                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 78:DS:181:GLN:NE2 | 78:DS:190:LEU:O    | 2.38                     | 0.57              |
| 12:r:53:VAL:HG21  | 12:r:166:ILE:HD12  | 1.86                     | 0.57              |
| 21:0:8:GLN:HB2    | 21:0:64:ILE:HD11   | 1.85                     | 0.57              |
| 25:7:108:LYS:HZ1  | 53:I:154:ARG:HD3   | 1.69                     | 0.57              |
| 59:O:132:GLU:HG3  | 59:O:133:ARG:H     | 1.70                     | 0.57              |
| 60:P:37:ILE:HG23  | 60:P:50:ILE:HG21   | 1.87                     | 0.57              |
| 64:T:14:LYS:HB2   | 64:T:69:ILE:HD11   | 1.87                     | 0.57              |
| 67:W:56:ARG:HG3   | 67:W:88:ARG:HH11   | 1.68                     | 0.57              |
| 1:AS:619:A:H2'    | 1:AS:620:A:C8      | 2.40                     | 0.57              |
| 1:AS:1034:U:H5''  | 7:AZ:5:LYS:HG2     | 1.86                     | 0.57              |
| 1:AS:2634:G:OP1   | 7:AZ:32:GLN:NE2    | 2.37                     | 0.57              |
| 4:AW:20:THR:HA    | 4:AW:23:ARG:HG3    | 1.85                     | 0.57              |
| 9:BB:185:GLU:HG2  | 9:BB:196:VAL:HG21  | 1.85                     | 0.57              |
| 23:BP:46:ILE:HD12 | 23:BP:47:VAL:H     | 1.69                     | 0.57              |
| 25:BR:1:MET:HE2   | 25:BR:15:PRO:HG2   | 1.87                     | 0.57              |
| 46:CM:870:G:H2'   | 46:CM:871:U:C6     | 2.39                     | 0.57              |
| 46:CM:1601:A:H5'  | 75:DP:47:PRO:HG3   | 1.87                     | 0.57              |
| 79:DT:159:PRO:CD  | 79:DT:201:LEU:HD12 | 2.35                     | 0.57              |
| 1:1:2244:U:H2'    | 1:1:2245:C:H6      | 1.69                     | 0.57              |
| 1:1:2492:U:OP2    | 1:1:2558:G:N2      | 2.37                     | 0.57              |
| 21:0:161:LYS:HB3  | 21:0:161:LYS:HZ2   | 1.70                     | 0.57              |
| 46:B:870:G:H2'    | 46:B:871:U:C6      | 2.40                     | 0.57              |
| 52:H:98:MET:O     | 52:H:99:MET:HE2    | 2.05                     | 0.57              |
| 78:h:157:GLU:HG2  | 78:h:159:LEU:HG    | 1.87                     | 0.57              |
| 79:AR:202:SER:O   | 79:AR:204:ASP:N    | 2.35                     | 0.57              |
| 5:AX:293:ASN:HB2  | 5:AX:304:THR:HA    | 1.87                     | 0.57              |
| 11:BD:47:LYS:HB2  | 15:BH:5:VAL:HB     | 1.86                     | 0.57              |
| 20:BM:53:LYS:HG2  | 20:BM:54:PRO:HD2   | 1.86                     | 0.57              |
| 26:BS:73:MET:HE2  | 26:BS:142:ILE:HB   | 1.87                     | 0.57              |
| 28:BU:27:LYS:HG2  | 28:BU:29:HIS:NE2   | 2.17                     | 0.57              |
| 46:CM:15:U:H2'    | 46:CM:16:G:O4'     | 2.05                     | 0.57              |
| 47:CN:13:ASP:CG   | 47:CN:179:ARG:HH22 | 2.13                     | 0.57              |
| 48:CO:128:LYS:NZ  | 48:CO:129:THR:O    | 2.30                     | 0.57              |
| 65:DF:126:ARG:HB2 | 65:DF:133:VAL:HG12 | 1.86                     | 0.57              |
| 66:DG:77:ASN:OD1  | 66:DG:101:ASN:ND2  | 2.30                     | 0.57              |
| 70:DK:107:PHE:HE1 | 70:DK:120:VAL:HG12 | 1.69                     | 0.57              |
| 79:DT:7:LEU:HA    | 79:DT:311:GLN:O    | 2.04                     | 0.57              |
| 27:9:39:LEU:HD22  | 27:9:43:TYR:HE2    | 1.68                     | 0.57              |
| 41:AN:22:LYS:HG3  | 41:AN:39:CYS:HB2   | 1.87                     | 0.57              |
| 46:B:219:A:H5''   | 46:B:818:U:H1'     | 1.86                     | 0.57              |
| 46:B:1132:A:H2'   | 46:B:1133:C:C6     | 2.40                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:J:13:LEU:HD21   | 54:J:54:LEU:HD11   | 1.86                     | 0.57              |
| 57:M:54:TYR:CE1    | 57:M:75:PHE:HB2    | 2.40                     | 0.57              |
| 5:AX:10:ARG:NH2    | 5:AX:263:THR:O     | 2.38                     | 0.57              |
| 21:BN:8:GLN:HB2    | 21:BN:64:ILE:HD11  | 1.86                     | 0.57              |
| 28:BU:70:PRO:HG3   | 28:BU:115:LYS:HB2  | 1.87                     | 0.57              |
| 46:CM:669:G:H2'    | 46:CM:671:G:C8     | 2.39                     | 0.57              |
| 46:CM:1715:U:H2'   | 46:CM:1716:C:C6    | 2.40                     | 0.57              |
| 54:CU:82:PRO:C     | 54:CU:84:ARG:H     | 2.12                     | 0.57              |
| 54:CU:85:HIS:HB3   | 54:CU:161:LYS:HD3  | 1.85                     | 0.57              |
| 69:DJ:11:LEU:HD11  | 69:DJ:37:PHE:CE2   | 2.35                     | 0.57              |
| 1:1:249:G:H2'      | 1:1:251:G:OP2      | 2.05                     | 0.57              |
| 1:1:269:G:H5''     | 16:v:14:LYS:HE2    | 1.85                     | 0.57              |
| 1:1:583:A:H2'      | 1:1:584:C:C6       | 2.40                     | 0.57              |
| 1:1:1761:U:C5      | 20:z:43:LYS:HE3    | 2.40                     | 0.57              |
| 1:1:2634:G:H2'     | 1:1:2635:A:C8      | 2.40                     | 0.57              |
| 8:n:39:LEU:HD11    | 8:n:53:TYR:HB2     | 1.86                     | 0.57              |
| 46:B:457:G:OP1     | 71:a:109:LYS:NZ    | 2.37                     | 0.57              |
| 46:B:924:A:H2'     | 46:B:925:A:C8      | 2.40                     | 0.57              |
| 46:B:1218:G:N1     | 46:B:1237:C:H5     | 2.01                     | 0.57              |
| 46:B:1454:U:O2'    | 66:V:87:GLY:O      | 2.21                     | 0.57              |
| 79:AR:40:LYS:HG2   | 79:AR:67:HIS:O     | 2.05                     | 0.57              |
| 1:AS:673:C:O2'     | 1:AS:677:U:OP1     | 2.22                     | 0.57              |
| 1:AS:2130:A:H2'    | 1:AS:2131:U:H6     | 1.70                     | 0.57              |
| 1:AS:2740:U:H2'    | 1:AS:2741:A:H8     | 1.70                     | 0.57              |
| 6:AY:284:ASN:HB3   | 6:AY:290:LEU:HD11  | 1.85                     | 0.57              |
| 15:BH:17:ARG:HD2   | 15:BH:61:VAL:HG22  | 1.86                     | 0.57              |
| 46:CM:504:A:H5''   | 46:CM:505:U:OP1    | 2.05                     | 0.57              |
| 46:CM:1302:C:H2'   | 46:CM:1303:G:O4'   | 2.05                     | 0.57              |
| 50:CQ:215:GLU:HG3  | 50:CQ:216:ASP:N    | 2.16                     | 0.57              |
| 51:CR:126:VAL:HG13 | 51:CR:139:VAL:HG13 | 1.87                     | 0.57              |
| 53:CT:180:THR:HG23 | 53:CT:183:THR:H    | 1.70                     | 0.57              |
| 59:CZ:121:VAL:HG22 | 59:CZ:122:VAL:H    | 1.69                     | 0.57              |
| 79:DT:103:ARG:HE   | 79:DT:105:VAL:HG22 | 1.70                     | 0.57              |
| 1:1:1746:A:H1'     | 1:1:1748:A:N7      | 2.20                     | 0.57              |
| 1:1:1810:A:H4'     | 1:1:1811:U:O4'     | 2.05                     | 0.57              |
| 1:1:3136:C:H2'     | 1:1:3137:A:H8      | 1.70                     | 0.57              |
| 1:1:3235:A:N6      | 18:x:178:SER:OG    | 2.38                     | 0.57              |
| 3:4:37:A:H5''      | 3:4:39:G:O4'       | 2.05                     | 0.57              |
| 13:s:61:ARG:NH2    | 45:i:43:PRO:HG2    | 2.19                     | 0.57              |
| 21:O:24:LEU:HD21   | 22:2:141:ILE:HG21  | 1.87                     | 0.57              |
| 46:B:248:C:H2'     | 46:B:249:A:H8      | 1.68                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:B:781:G:H4'     | 58:N:69:LYS:NZ     | 2.20                     | 0.57              |
| 46:B:1635:A:H2'    | 46:B:1636:C:C6     | 2.40                     | 0.57              |
| 50:F:56:THR:O      | 50:F:60:LEU:HG     | 2.05                     | 0.57              |
| 57:M:70:ASP:O      | 57:M:73:VAL:HG22   | 2.05                     | 0.57              |
| 68:X:64:GLU:OE2    | 74:d:2:VAL:N       | 2.37                     | 0.57              |
| 69:Y:28:ARG:HD3    | 69:Y:60:LYS:HE2    | 1.87                     | 0.57              |
| 1:AS:112:C:OP1     | 16:BI:147:ARG:NH2  | 2.38                     | 0.57              |
| 1:AS:169:G:H1      | 1:AS:248:U:H3      | 1.53                     | 0.57              |
| 1:AS:1303:G:OP1    | 17:BJ:60:ARG:NH2   | 2.38                     | 0.57              |
| 1:AS:2912:A:OP2    | 5:AX:2:SER:N       | 2.38                     | 0.57              |
| 1:AS:3064:C:O2'    | 1:AS:3066:A:OP2    | 2.19                     | 0.57              |
| 1:AS:3138:U:H2'    | 1:AS:3139:U:C6     | 2.40                     | 0.57              |
| 3:AU:71:A:N1       | 3:AU:82:U:O2'      | 2.36                     | 0.57              |
| 5:AX:136:LYS:HG2   | 5:AX:143:GLN:OE1   | 2.04                     | 0.57              |
| 23:BP:101:VAL:HG23 | 23:BP:102:LYS:H    | 1.70                     | 0.57              |
| 26:BS:58:ASP:O     | 26:BS:62:ILE:HG13  | 2.05                     | 0.57              |
| 29:BV:112:VAL:HB   | 29:BV:130:VAL:HG12 | 1.86                     | 0.57              |
| 46:CM:165:U:H4'    | 53:CT:134:GLY:O    | 2.04                     | 0.57              |
| 48:CO:30:PHE:CZ    | 48:CO:61:LEU:HD11  | 2.40                     | 0.57              |
| 50:CQ:214:ASP:CG   | 50:CQ:215:GLU:H    | 2.11                     | 0.57              |
| 79:DT:12:THR:HA    | 79:DT:308:ARG:HA   | 1.87                     | 0.57              |
| 81:P0:6:GLU:OE1    | 81:P0:6:GLU:N      | 2.29                     | 0.57              |
| 1:1:534:G:H1       | 1:1:551:U:H3       | 1.51                     | 0.56              |
| 1:1:1241:A:H3'     | 1:1:1242:G:H5''    | 1.85                     | 0.56              |
| 1:1:1251:C:H2'     | 1:1:1252:G:C8      | 2.40                     | 0.56              |
| 1:1:1456:A:H2'     | 1:1:1457:A:H8      | 1.68                     | 0.56              |
| 1:1:1663:A:H2'     | 1:1:1664:G:H8      | 1.69                     | 0.56              |
| 1:1:2796:G:H2'     | 1:1:2797:C:H6      | 1.69                     | 0.56              |
| 46:B:1283:U:H2'    | 46:B:1284:G:O4'    | 2.04                     | 0.56              |
| 63:S:67:LYS:O      | 63:S:67:LYS:HG2    | 2.05                     | 0.56              |
| 79:AR:200:THR:HG21 | 79:AR:241:ALA:HA   | 1.87                     | 0.56              |
| 1:AS:638:U:OP1     | 29:BV:21:ARG:NH1   | 2.36                     | 0.56              |
| 1:AS:788:G:H2'     | 1:AS:789:C:C6      | 2.40                     | 0.56              |
| 1:AS:1190:G:H2'    | 1:AS:1191:A:C8     | 2.40                     | 0.56              |
| 17:BJ:125:LEU:HD13 | 21:BN:168:PRO:HG3  | 1.87                     | 0.56              |
| 28:BU:33:THR:HG23  | 28:BU:34:LYS:O     | 2.05                     | 0.56              |
| 46:CM:151:G:O6     | 71:DL:128:ARG:NH2  | 2.25                     | 0.56              |
| 46:CM:1413:A:O2'   | 46:CM:1414:G:OP1   | 2.21                     | 0.56              |
| 55:CV:65:PHE:CZ    | 55:CV:78:ILE:HD11  | 2.40                     | 0.56              |
| 61:DB:55:ALA:HB1   | 61:DB:96:ALA:HB2   | 1.86                     | 0.56              |
| 63:DD:89:VAL:HG13  | 63:DD:101:LYS:HG2  | 1.85                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 66:DG:117:SER:HB2 | 66:DG:123:ARG:H   | 1.69                     | 0.56              |
| 67:DH:68:LYS:HE2  | 67:DH:79:ASP:OD1  | 2.05                     | 0.56              |
| 71:DL:6:THR:HB    | 71:DL:28:LEU:HB2  | 1.87                     | 0.56              |
| 79:DT:234:LYS:HG3 | 79:DT:258:LYS:HE3 | 1.87                     | 0.56              |
| 82:12:137:GLN:HB3 | 82:12:148:PRO:HB2 | 1.87                     | 0.56              |
| 1:1:93:G:H2'      | 1:1:94:A:C8       | 2.39                     | 0.56              |
| 1:1:563:U:H2'     | 1:1:564:G:C8      | 2.40                     | 0.56              |
| 1:1:907:C:N4      | 4:j:3:ARG:HD3     | 2.21                     | 0.56              |
| 9:o:149:ARG:HD2   | 9:o:205:LEU:HD23  | 1.87                     | 0.56              |
| 13:s:110:ILE:HG21 | 13:s:116:TYR:HD2  | 1.69                     | 0.56              |
| 25:7:107:SER:O    | 25:7:111:LYS:HG2  | 2.04                     | 0.56              |
| 46:B:137:A:O4'    | 46:B:139:U:H5'    | 2.05                     | 0.56              |
| 46:B:510:A:O2'    | 56:L:133:HIS:NE2  | 2.26                     | 0.56              |
| 46:B:1301:G:OP1   | 64:T:7:LYS:N      | 2.36                     | 0.56              |
| 46:B:1410:A:H2'   | 49:E:87:ALA:CB    | 2.34                     | 0.56              |
| 46:B:1566:U:H1'   | 63:S:138:GLN:HG3  | 1.87                     | 0.56              |
| 50:F:224:VAL:HG23 | 79:AR:188:ASP:HB2 | 1.87                     | 0.56              |
| 66:V:53:TRP:HH2   | 66:V:100:ILE:HD12 | 1.69                     | 0.56              |
| 1:AS:314:U:H2'    | 1:AS:315:C:C6     | 2.39                     | 0.56              |
| 1:AS:951:U:H2'    | 1:AS:952:U:C6     | 2.40                     | 0.56              |
| 1:AS:1124:U:OP1   | 80:BE:4:ARG:NH1   | 2.35                     | 0.56              |
| 1:AS:1302:G:N2    | 1:AS:1303:G:N7    | 2.53                     | 0.56              |
| 1:AS:2086:C:H1'   | 1:AS:3309:A:H8    | 1.68                     | 0.56              |
| 2:AT:53:U:O2'     | 2:AT:55:A:N7      | 2.39                     | 0.56              |
| 46:CM:654:G:H8    | 46:CM:654:G:O5'   | 1.88                     | 0.56              |
| 46:CM:829:A:H2'   | 46:CM:830:G:C8    | 2.40                     | 0.56              |
| 79:DT:107:HIS:NE2 | 79:DT:127:SER:HB3 | 2.21                     | 0.56              |
| 1:1:208:A:OP1     | 6:l:162:LYS:NZ    | 2.31                     | 0.56              |
| 1:1:1253:C:H5'    | 1:1:1254:U:OP2    | 2.05                     | 0.56              |
| 1:1:1596:U:H5''   | 20:z:42:ARG:NH2   | 2.19                     | 0.56              |
| 1:1:2445:G:O2'    | 1:1:2446:A:O5'    | 2.21                     | 0.56              |
| 1:1:2700:G:N7     | 22:2:87:LYS:NZ    | 2.45                     | 0.56              |
| 1:1:3241:G:O2'    | 18:x:175:ARG:HD3  | 2.05                     | 0.56              |
| 13:s:52:TYR:CD2   | 45:i:48:PRO:HA    | 2.39                     | 0.56              |
| 23:5:34:VAL:HG21  | 23:5:58:ALA:HB2   | 1.88                     | 0.56              |
| 25:7:87:LEU:HA    | 25:7:90:ILE:HD12  | 1.87                     | 0.56              |
| 25:7:123:ARG:HH21 | 46:B:270:U:H4'    | 1.68                     | 0.56              |
| 27:9:58:VAL:HA    | 27:9:104:VAL:HG12 | 1.86                     | 0.56              |
| 36:AI:5:LYS:O     | 36:AI:9:LEU:HG    | 2.04                     | 0.56              |
| 43:AP:8:ARG:HG2   | 43:AP:10:THR:HG23 | 1.86                     | 0.56              |
| 46:B:151:G:H2'    | 46:B:152:G:C8     | 2.40                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:B:874:U:H2'     | 46:B:875:C:H6      | 1.70                     | 0.56              |
| 46:B:932:U:H2'     | 46:B:933:A:C8      | 2.40                     | 0.56              |
| 46:B:1312:C:O2'    | 50:F:160:HIS:ND1   | 2.36                     | 0.56              |
| 46:B:1578:C:H2'    | 46:B:1579:A:C8     | 2.41                     | 0.56              |
| 53:I:68:MET:O      | 53:I:69:HIS:ND1    | 2.37                     | 0.56              |
| 56:L:110:GLN:NE2   | 56:L:126:ARG:HB2   | 2.20                     | 0.56              |
| 62:R:14:GLN:OE1    | 62:R:22:LEU:N      | 2.38                     | 0.56              |
| 69:Y:77:PRO:HD2    | 69:Y:79:PHE:CZ     | 2.40                     | 0.56              |
| 78:h:167:THR:HG21  | 78:h:186:CYS:HB3   | 1.87                     | 0.56              |
| 1:AS:269:G:N2      | 1:AS:295:A:OP2     | 2.23                     | 0.56              |
| 1:AS:293:C:O2'     | 37:CD:75:ARG:HA    | 2.04                     | 0.56              |
| 1:AS:307:A:H2'     | 1:AS:308:A:H8      | 1.70                     | 0.56              |
| 1:AS:907:C:H42     | 4:AW:3:ARG:HD3     | 1.69                     | 0.56              |
| 1:AS:1456:A:H2'    | 1:AS:1457:A:C8     | 2.41                     | 0.56              |
| 1:AS:1575:A:OP1    | 1:AS:2500:G:N2     | 2.38                     | 0.56              |
| 1:AS:1795:A:H2'    | 1:AS:1796:A:H8     | 1.69                     | 0.56              |
| 1:AS:3132:U:H2'    | 1:AS:3133:G:C8     | 2.40                     | 0.56              |
| 2:AT:113:C:H2'     | 2:AT:114:U:O4'     | 2.05                     | 0.56              |
| 5:AX:66:LYS:HZ1    | 24:BQ:9:ASN:H      | 1.52                     | 0.56              |
| 10:BC:156:ASN:HD21 | 10:BC:182:LYS:HG3  | 1.70                     | 0.56              |
| 22:BO:116:LYS:HG2  | 22:BO:120:LYS:HD2  | 1.87                     | 0.56              |
| 28:BU:57:MET:CB    | 28:BU:61:LYS:HE2   | 2.35                     | 0.56              |
| 28:BU:108:GLU:HG3  | 28:BU:112:LYS:HE3  | 1.87                     | 0.56              |
| 45:CL:120:GLU:HB3  | 50:CQ:118:ARG:HG3  | 1.86                     | 0.56              |
| 46:CM:698:C:H2'    | 46:CM:699:U:C6     | 2.40                     | 0.56              |
| 46:CM:721:C:H42    | 46:CM:722:A:H62    | 1.53                     | 0.56              |
| 46:CM:1055:A:H4'   | 74:DO:17:LYS:HE3   | 1.87                     | 0.56              |
| 46:CM:1265:C:O2'   | 67:DH:69:THR:HG22  | 2.05                     | 0.56              |
| 46:CM:1315:G:H2'   | 46:CM:1316:A:O4'   | 2.05                     | 0.56              |
| 46:CM:1354:U:N3    | 46:CM:1355:A:N7    | 2.53                     | 0.56              |
| 47:CN:88:LYS:HD2   | 47:CN:201:LEU:HD11 | 1.86                     | 0.56              |
| 48:CO:86:LEU:HB3   | 48:CO:98:THR:HB    | 1.88                     | 0.56              |
| 48:CO:135:LEU:HD21 | 48:CO:184:LEU:HD21 | 1.87                     | 0.56              |
| 48:CO:144:LYS:HD3  | 48:CO:207:LEU:O    | 2.04                     | 0.56              |
| 52:CS:143:ARG:HH21 | 52:CS:214:LYS:HD3  | 1.69                     | 0.56              |
| 54:CU:70:GLN:O     | 54:CU:74:THR:OG1   | 2.23                     | 0.56              |
| 54:CU:136:VAL:HB   | 69:DJ:52:TYR:HB3   | 1.87                     | 0.56              |
| 57:CX:15:LEU:HD23  | 57:CX:76:LEU:HD11  | 1.88                     | 0.56              |
| 58:CY:7:VAL:HG12   | 58:CY:53:TYR:HA    | 1.88                     | 0.56              |
| 59:CZ:47:GLU:HA    | 59:CZ:50:LYS:HZ3   | 1.70                     | 0.56              |
| 59:CZ:94:ALA:C     | 59:CZ:95:LYS:HG3   | 2.30                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:DT:46:LYS:CB    | 79:DT:57:ILE:HG22  | 2.34                     | 0.56              |
| 79:DT:67:HIS:HB3   | 79:DT:86:TRP:HB2   | 1.86                     | 0.56              |
| 79:DT:101:THR:HG22 | 79:DT:102:GLN:N    | 2.21                     | 0.56              |
| 79:DT:203:PRO:HG2  | 79:DT:247:TYR:HE1  | 1.70                     | 0.56              |
| 81:P0:25:ILE:HD12  | 81:P0:88:PHE:HA    | 1.86                     | 0.56              |
| 1:1:627:U:H2'      | 1:1:628:A:H8       | 1.67                     | 0.56              |
| 1:1:1060:A:H4'     | 1:1:1061:A:O5'     | 2.05                     | 0.56              |
| 1:1:1674:G:O6      | 23:5:77:LYS:NZ     | 2.31                     | 0.56              |
| 1:1:2361:C:OP2     | 17:w:86:ARG:NH2    | 2.25                     | 0.56              |
| 1:1:2443:G:O2'     | 1:1:2444:G:OP1     | 2.15                     | 0.56              |
| 1:1:2854:U:H2'     | 1:1:2855:U:C6      | 2.40                     | 0.56              |
| 46:B:472:A:H5''    | 56:L:144:PRO:HD2   | 1.86                     | 0.56              |
| 46:B:681:C:H3'     | 46:B:682:A:H8      | 1.69                     | 0.56              |
| 1:AS:582:G:H2'     | 1:AS:583:A:H8      | 1.70                     | 0.56              |
| 1:AS:1225:G:H2'    | 1:AS:1226:G:H8     | 1.70                     | 0.56              |
| 1:AS:1720:U:H1'    | 1:AS:1721:C:C6     | 2.40                     | 0.56              |
| 1:AS:2419:A:H2'    | 1:AS:2420:G:C8     | 2.40                     | 0.56              |
| 15:BH:65:LEU:HD12  | 15:BH:77:LYS:HD2   | 1.88                     | 0.56              |
| 36:CC:100:GLU:OE2  | 36:CC:108:ARG:NH2  | 2.35                     | 0.56              |
| 46:CM:1050:A:H5'   | 48:CO:160:LYS:HZ1  | 1.70                     | 0.56              |
| 46:CM:1241:A:H5'   | 46:CM:1242:U:C5    | 2.40                     | 0.56              |
| 46:CM:1265:C:H2'   | 46:CM:1266:G:H8    | 1.71                     | 0.56              |
| 46:CM:1410:A:C2'   | 49:CP:87:ALA:HB3   | 2.33                     | 0.56              |
| 47:CN:48:ILE:HG12  | 47:CN:149:MET:HE3  | 1.88                     | 0.56              |
| 48:CO:30:PHE:HE1   | 48:CO:46:THR:HG1   | 1.52                     | 0.56              |
| 54:CU:118:HIS:CG   | 54:CU:175:LYS:HZ1  | 2.23                     | 0.56              |
| 62:DC:69:PRO:HB2   | 62:DC:71:GLU:OE1   | 2.05                     | 0.56              |
| 67:DH:43:ASN:HD21  | 67:DH:105:ILE:HG21 | 1.70                     | 0.56              |
| 79:DT:101:THR:HG22 | 79:DT:102:GLN:H    | 1.70                     | 0.56              |
| 1:1:2330:A:H5''    | 18:x:83:TRP:O      | 2.04                     | 0.56              |
| 1:1:3021:A:N1      | 24:6:86:ARG:NH2    | 2.52                     | 0.56              |
| 25:7:105:ARG:CZ    | 53:I:151:ASP:HA    | 2.36                     | 0.56              |
| 45:i:92:SER:OG     | 45:i:94:THR:HG22   | 2.06                     | 0.56              |
| 46:B:209:U:H5''    | 58:N:20:PHE:CG     | 2.39                     | 0.56              |
| 46:B:338:U:H2'     | 46:B:339:A:C8      | 2.41                     | 0.56              |
| 46:B:1020:G:OP1    | 60:P:2:GLY:N       | 2.38                     | 0.56              |
| 50:F:106:LEU:HD21  | 50:F:139:ILE:HD11  | 1.87                     | 0.56              |
| 1:AS:88:G:N7       | 19:BL:171:LYS:NZ   | 2.53                     | 0.56              |
| 1:AS:172:C:O2'     | 1:AS:173:C:OP1     | 2.21                     | 0.56              |
| 1:AS:1148:G:N2     | 1:AS:1148:G:OP2    | 2.39                     | 0.56              |
| 1:AS:1526:U:O3'    | 3:AU:114:G:O2'     | 2.22                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:3135:A:H2'    | 1:AS:3136:C:H6     | 1.69                     | 0.56              |
| 5:AX:106:TRP:HB2   | 5:AX:133:TYR:CE1   | 2.40                     | 0.56              |
| 14:BG:69:VAL:HG11  | 14:BG:152:PRO:HD3  | 1.87                     | 0.56              |
| 46:CM:678:A:OP1    | 46:CM:678:A:H4'    | 2.05                     | 0.56              |
| 48:CO:57:ALA:O     | 48:CO:61:LEU:HB3   | 2.05                     | 0.56              |
| 79:DT:198:CYS:SG   | 79:DT:239:ALA:HA   | 2.46                     | 0.56              |
| 1:1:157:G:H2'      | 1:1:158:A:H8       | 1.70                     | 0.56              |
| 1:1:981:U:H5''     | 9:o:96:LYS:HE2     | 1.88                     | 0.56              |
| 15:u:15:VAL:HG11   | 15:u:67:ARG:HA     | 1.87                     | 0.56              |
| 17:w:76:ALA:HB3    | 17:w:79:ARG:HG2    | 1.87                     | 0.56              |
| 1:AS:139:U:H2'     | 1:AS:140:C:C6      | 2.40                     | 0.56              |
| 1:AS:357:A:O4'     | 6:AY:82:GLY:HA3    | 2.06                     | 0.56              |
| 1:AS:1060:A:H4'    | 1:AS:1061:A:O5'    | 2.06                     | 0.56              |
| 1:AS:1489:G:N2     | 1:AS:1489:G:OP2    | 2.35                     | 0.56              |
| 1:AS:2719:A:H5'    | 7:AZ:175:HIS:HA    | 1.87                     | 0.56              |
| 1:AS:3088:G:H4'    | 11:BD:69:ARG:NH1   | 2.20                     | 0.56              |
| 6:AY:301:ARG:NH2   | 19:BL:38:ARG:O     | 2.38                     | 0.56              |
| 28:BU:109:GLU:O    | 28:BU:113:VAL:HG23 | 2.05                     | 0.56              |
| 34:CA:42:LYS:HA    | 34:CA:45:LEU:HG    | 1.87                     | 0.56              |
| 35:CB:99:LYS:O     | 35:CB:103:ARG:HG3  | 2.05                     | 0.56              |
| 45:CL:161:SER:O    | 45:CL:164:GLU:HB2  | 2.05                     | 0.56              |
| 46:CM:1659:G:H2'   | 46:CM:1660:G:H8    | 1.69                     | 0.56              |
| 51:CR:123:LEU:HD23 | 51:CR:159:THR:HG21 | 1.87                     | 0.56              |
| 54:CU:25:GLU:OE2   | 54:CU:25:GLU:N     | 2.36                     | 0.56              |
| 1:1:164:U:H2'      | 1:1:165:C:H6       | 1.70                     | 0.56              |
| 1:1:820:C:H5''     | 4:j:21:ARG:HD3     | 1.87                     | 0.56              |
| 1:1:2634:G:H2'     | 1:1:2635:A:H8      | 1.69                     | 0.56              |
| 7:m:132:THR:HG21   | 7:m:170:GLY:O      | 2.05                     | 0.56              |
| 22:2:82:ASN:HB2    | 30:AC:20:GLY:HA3   | 1.88                     | 0.56              |
| 46:B:1134:G:H1     | 46:B:1615:U:H3     | 1.53                     | 0.56              |
| 47:C:184:LEU:HB3   | 68:X:45:ALA:HB2    | 1.88                     | 0.56              |
| 59:O:96:LEU:HD12   | 59:O:100:TRP:CZ3   | 2.40                     | 0.56              |
| 67:W:34:GLU:OE2    | 67:W:88:ARG:NH2    | 2.38                     | 0.56              |
| 79:AR:26:THR:HG23  | 79:AR:29:HIS:H     | 1.70                     | 0.56              |
| 1:AS:45:U:O4       | 16:BI:83:LYS:NZ    | 2.37                     | 0.56              |
| 1:AS:834:G:O6      | 44:CK:4:ARG:NH2    | 2.38                     | 0.56              |
| 1:AS:844:A:C5      | 1:AS:845:C:H1'     | 2.41                     | 0.56              |
| 1:AS:2587:G:H2'    | 1:AS:2588:C:H6     | 1.70                     | 0.56              |
| 83:AS:3401:3K5:H7  | 83:AS:3401:3K5:H11 | 1.86                     | 0.56              |
| 38:CE:21:ARG:HD2   | 38:CE:37:CYS:SG    | 2.45                     | 0.56              |
| 45:CL:71:LYS:NZ    | 62:DC:126:VAL:O    | 2.33                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:CO:68:VAL:HG22  | 48:CO:69:CYS:H    | 1.71                     | 0.56              |
| 48:CO:131:ASP:HB3  | 48:CO:180:THR:CG2 | 2.34                     | 0.56              |
| 54:CU:173:THR:HB   | 54:CU:175:LYS:HZ2 | 1.71                     | 0.56              |
| 1:1:941:C:H2'      | 1:1:942:U:C6      | 2.41                     | 0.56              |
| 1:1:1018:U:H2'     | 1:1:1019:U:C6     | 2.41                     | 0.56              |
| 3:4:85:G:O6        | 27:9:114:ASP:N    | 2.38                     | 0.56              |
| 5:k:95:THR:OG1     | 5:k:98:GLY:O      | 2.21                     | 0.56              |
| 5:k:339:ARG:NH2    | 5:k:342:LEU:HD11  | 2.20                     | 0.56              |
| 46:B:226:G:H2'     | 46:B:227:C:C6     | 2.40                     | 0.56              |
| 46:B:786:G:H21     | 69:Y:107:SER:HB3  | 1.71                     | 0.56              |
| 46:B:1423:U:O2'    | 50:F:182:VAL:HG23 | 2.06                     | 0.56              |
| 46:B:1479:A:H4'    | 46:B:1480:G:O5'   | 2.06                     | 0.56              |
| 46:B:1485:G:H2'    | 46:B:1486:G:H8    | 1.70                     | 0.56              |
| 46:B:1512:A:H2'    | 46:B:1513:A:C8    | 2.41                     | 0.56              |
| 46:B:1566:U:H2'    | 46:B:1567:C:C6    | 2.41                     | 0.56              |
| 50:F:193:PRO:HG3   | 50:F:203:LEU:HD12 | 1.87                     | 0.56              |
| 1:AS:530:U:OP1     | 21:BN:132:THR:OG1 | 2.19                     | 0.56              |
| 1:AS:1034:U:H1'    | 7:AZ:3:MET:HE3    | 1.87                     | 0.56              |
| 1:AS:1653:C:O2'    | 1:AS:1793:A:OP2   | 2.21                     | 0.56              |
| 1:AS:1943:G:O2'    | 1:AS:1944:G:OP1   | 2.20                     | 0.56              |
| 13:BF:101:ASN:HD22 | 13:BF:131:MET:H   | 1.52                     | 0.56              |
| 46:CM:39:A:OP1     | 56:CW:3:ARG:NH2   | 2.38                     | 0.56              |
| 46:CM:184:C:H2'    | 46:CM:185:G:O4'   | 2.05                     | 0.56              |
| 46:CM:261:C:H4'    | 46:CM:290:U:H5'   | 1.87                     | 0.56              |
| 46:CM:1131:G:H2'   | 46:CM:1132:A:C8   | 2.41                     | 0.56              |
| 46:CM:1463:G:H2'   | 46:CM:1464:G:H8   | 1.70                     | 0.56              |
| 79:DT:107:HIS:CE1  | 79:DT:127:SER:HB3 | 2.41                     | 0.56              |
| 1:1:255:A:H5'      | 36:AI:106:LYS:HD3 | 1.87                     | 0.56              |
| 1:1:783:G:H2'      | 1:1:784:C:H6      | 1.71                     | 0.56              |
| 3:4:81:A:H2'       | 3:4:82:U:C6       | 2.41                     | 0.56              |
| 8:n:7:LYS:H        | 8:n:10:GLN:HG3    | 1.71                     | 0.56              |
| 14:t:122:LYS:HB3   | 36:AI:119:LYS:H   | 1.69                     | 0.56              |
| 46:B:871:U:H2'     | 46:B:872:A:H8     | 1.71                     | 0.56              |
| 46:B:1508:G:O2'    | 46:B:1510:G:OP2   | 2.21                     | 0.56              |
| 47:C:134:LYS:HE3   | 47:C:138:TYR:HE1  | 1.71                     | 0.56              |
| 1:AS:1400:G:N2     | 1:AS:1403:A:OP2   | 2.29                     | 0.56              |
| 1:AS:2138:G:H2'    | 1:AS:2139:G:H8    | 1.70                     | 0.56              |
| 10:BC:61:ARG:O     | 10:BC:65:ILE:HD12 | 2.05                     | 0.56              |
| 45:CL:61:GLU:C     | 45:CL:63:ALA:H    | 2.14                     | 0.56              |
| 46:CM:136:U:O2'    | 53:CT:149:LYS:NZ  | 2.26                     | 0.56              |
| 46:CM:985:C:H5     | 46:CM:988:A:H5''  | 1.71                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:CO:138:PHE:CD1 | 48:CO:214:LYS:HG3  | 2.41                     | 0.56              |
| 48:CO:197:ILE:O   | 48:CO:201:THR:HG23 | 2.05                     | 0.56              |
| 59:CZ:90:LYS:HG2  | 59:CZ:91:VAL:N     | 2.21                     | 0.56              |
| 65:DF:132:LYS:NZ  | 65:DF:141:THR:OG1  | 2.39                     | 0.56              |
| 69:DJ:11:LEU:HD12 | 69:DJ:74:VAL:HG13  | 1.87                     | 0.56              |
| 79:DT:48:THR:N    | 79:DT:55:TYR:O     | 2.36                     | 0.56              |
| 1:1:447:U:H3      | 1:1:483:U:H3       | 1.53                     | 0.56              |
| 1:1:782:A:H4'     | 1:1:783:G:H5'      | 1.88                     | 0.56              |
| 1:1:1059:G:N7     | 1:1:1093:G:O2'     | 2.32                     | 0.56              |
| 1:1:1611:U:H2'    | 1:1:1612:U:C6      | 2.41                     | 0.56              |
| 1:1:1642:G:O2'    | 1:1:1804:G:N2      | 2.35                     | 0.56              |
| 1:1:2196:G:H2'    | 1:1:2197:A:C8      | 2.39                     | 0.56              |
| 1:1:3316:U:H3     | 55:K:110:ARG:HH12  | 1.54                     | 0.56              |
| 2:3:64:A:H61      | 12:r:200:LEU:HD21  | 1.71                     | 0.56              |
| 68:X:73:ALA:HB1   | 68:X:78:LEU:HB2    | 1.88                     | 0.56              |
| 1:AS:96:U:OP2     | 14:BG:13:HIS:ND1   | 2.39                     | 0.56              |
| 1:AS:273:A:H2'    | 1:AS:274:G:C8      | 2.41                     | 0.56              |
| 1:AS:2766:G:N3    | 83:AS:3401:3K5:H1  | 2.21                     | 0.56              |
| 4:AW:36:GLU:OE1   | 4:AW:163:ARG:NH1   | 2.38                     | 0.56              |
| 23:BP:19:VAL:CG1  | 23:BP:23:VAL:HG23  | 2.36                     | 0.56              |
| 46:CM:673:A:H2'   | 46:CM:674:C:C6     | 2.42                     | 0.56              |
| 46:CM:1602:C:N4   | 52:CS:80:LYS:O     | 2.39                     | 0.56              |
| 54:CU:30:LEU:HB2  | 54:CU:34:LEU:HD13  | 1.87                     | 0.56              |
| 82:12:120:SER:C   | 82:12:122:GLY:H    | 2.14                     | 0.56              |
| 1:1:1225:G:H4'    | 81:P0:32:ASN:OD1   | 2.06                     | 0.55              |
| 1:1:1434:U:H4'    | 6:l:89:ALA:HB3     | 1.89                     | 0.55              |
| 1:1:1789:C:O2     | 4:j:188:LYS:NZ     | 2.24                     | 0.55              |
| 3:4:21:C:H5''     | 6:l:195:LEU:HD21   | 1.88                     | 0.55              |
| 21:0:60:SER:OG    | 21:0:62:ASN:ND2    | 2.38                     | 0.55              |
| 46:B:470:U:O2'    | 46:B:754:A:N3      | 2.35                     | 0.55              |
| 46:B:733:U:OP1    | 69:Y:82:LYS:NZ     | 2.40                     | 0.55              |
| 46:B:1118:A:N3    | 46:B:1637:U:O2'    | 2.37                     | 0.55              |
| 46:B:1315:G:H21   | 64:T:8:THR:HG21    | 1.70                     | 0.55              |
| 46:B:1432:A:O2'   | 46:B:1433:C:H5''   | 2.05                     | 0.55              |
| 46:B:1743:A:H5''  | 46:B:1743:A:H8     | 1.70                     | 0.55              |
| 50:F:62:GLU:HB3   | 50:F:65:ARG:NH2    | 2.21                     | 0.55              |
| 53:I:116:GLN:NE2  | 53:I:125:THR:HB    | 2.20                     | 0.55              |
| 1:AS:605:U:OP2    | 8:BA:21:ARG:HG2    | 2.07                     | 0.55              |
| 1:AS:3166:A:C2    | 1:AS:3167:G:N7     | 2.75                     | 0.55              |
| 1:AS:3237:C:OP2   | 8:BA:77:ARG:NE     | 2.39                     | 0.55              |
| 11:BD:2:LYS:HD3   | 11:BD:61:ASP:OD1   | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:BD:76:ALA:O     | 11:BD:79:ILE:HG22  | 2.05                     | 0.55              |
| 28:BU:40:HIS:CD2   | 28:BU:74:LEU:HD11  | 2.40                     | 0.55              |
| 50:CQ:216:ASP:OD2  | 79:DT:173:LYS:NZ   | 2.38                     | 0.55              |
| 59:CZ:133:ARG:NH2  | 59:CZ:134:ASN:HD21 | 2.04                     | 0.55              |
| 62:DC:33:PHE:HB2   | 62:DC:87:PRO:HG2   | 1.87                     | 0.55              |
| 64:DE:69:ILE:HG13  | 64:DE:69:ILE:O     | 2.06                     | 0.55              |
| 81:P0:7:LYS:HA     | 81:P0:10:GLN:HB2   | 1.88                     | 0.55              |
| 81:P0:63:ILE:HA    | 81:P0:66:PHE:HB2   | 1.87                     | 0.55              |
| 1:1:2186:A:O2'     | 1:1:2187:U:H5'     | 2.06                     | 0.55              |
| 5:k:29:VAL:HG13    | 5:k:339:ARG:HD3    | 1.87                     | 0.55              |
| 14:t:46:ILE:O      | 14:t:49:ARG:HB2    | 2.06                     | 0.55              |
| 46:B:82:U:H2'      | 46:B:83:G:O4'      | 2.05                     | 0.55              |
| 46:B:1413:A:O2'    | 46:B:1414:G:OP1    | 2.24                     | 0.55              |
| 46:B:1463:G:H2'    | 46:B:1464:G:C8     | 2.41                     | 0.55              |
| 46:B:1533:G:OP1    | 65:U:123:ARG:NH1   | 2.37                     | 0.55              |
| 54:J:150:LEU:HB2   | 54:J:181:ILE:HG12  | 1.88                     | 0.55              |
| 59:O:47:GLU:HA     | 59:O:50:LYS:HG2    | 1.89                     | 0.55              |
| 79:AR:160:SER:HB3  | 79:AR:204:ASP:O    | 2.06                     | 0.55              |
| 3:AU:80:U:H3'      | 36:CC:43:ARG:NH2   | 2.20                     | 0.55              |
| 10:BC:151:LEU:HD22 | 10:BC:216:ILE:HD12 | 1.88                     | 0.55              |
| 46:CM:573:C:N4     | 70:DK:65:ASN:OD1   | 2.36                     | 0.55              |
| 46:CM:638:U:O2     | 54:CU:175:LYS:HE3  | 2.06                     | 0.55              |
| 55:CV:57:ALA:HB2   | 55:CV:183:GLY:HA2  | 1.88                     | 0.55              |
| 60:DA:110:ASP:O    | 60:DA:114:ARG:HG2  | 2.06                     | 0.55              |
| 63:DD:22:LYS:HG2   | 63:DD:63:ASP:OD1   | 2.06                     | 0.55              |
| 75:DP:42:ARG:NH1   | 75:DP:58:GLU:O     | 2.39                     | 0.55              |
| 81:P0:16:ARG:NH1   | 81:P0:63:ILE:HG12  | 2.21                     | 0.55              |
| 1:1:21:G:H5''      | 38:AK:43:LYS:HG2   | 1.89                     | 0.55              |
| 1:1:481:G:H2'      | 1:1:482:U:C6       | 2.41                     | 0.55              |
| 1:1:496:A:H2'      | 1:1:497:U:C6       | 2.42                     | 0.55              |
| 1:1:1322:A:O2'     | 34:AG:77:ASN:OD1   | 2.22                     | 0.55              |
| 45:i:91:HIS:O      | 46:B:1259:C:N4     | 2.39                     | 0.55              |
| 46:B:1495:U:H2'    | 46:B:1496:C:C6     | 2.41                     | 0.55              |
| 51:G:100:ARG:NH2   | 51:G:121:TYR:O     | 2.37                     | 0.55              |
| 1:AS:340:C:O2'     | 1:AS:344:A:N3      | 2.36                     | 0.55              |
| 1:AS:960:G:OP2     | 1:AS:1111:G:N1     | 2.38                     | 0.55              |
| 1:AS:2852:U:H1'    | 5:AX:250:ALA:HB3   | 1.87                     | 0.55              |
| 1:AS:3165:U:H2'    | 1:AS:3166:A:O4'    | 2.06                     | 0.55              |
| 4:AW:54:ARG:HH21   | 4:AW:58:LEU:HD11   | 1.70                     | 0.55              |
| 4:AW:180:LEU:HD23  | 44:CK:18:TYR:CD2   | 2.41                     | 0.55              |
| 8:BA:39:LEU:HD11   | 8:BA:53:TYR:HB2    | 1.88                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:CM:1149:G:O2'   | 46:CM:1599:U:O2   | 2.21                     | 0.55              |
| 46:CM:1445:C:OP1   | 65:DF:126:ARG:NH1 | 2.39                     | 0.55              |
| 48:CO:66:PHE:CE2   | 61:DB:29:SER:CB   | 2.83                     | 0.55              |
| 52:CS:200:ASN:HB3  | 52:CS:205:SER:HB3 | 1.87                     | 0.55              |
| 53:CT:159:ARG:NH1  | 53:CT:170:THR:OG1 | 2.40                     | 0.55              |
| 70:DK:19:ARG:O     | 70:DK:23:ARG:HG3  | 2.06                     | 0.55              |
| 71:DL:74:LEU:HD13  | 71:DL:76:TYR:CE1  | 2.40                     | 0.55              |
| 79:DT:89:THR:HG22  | 79:DT:105:VAL:HA  | 1.88                     | 0.55              |
| 1:1:25:A:H2'       | 1:1:26:C:H6       | 1.72                     | 0.55              |
| 1:1:538:G:H1       | 1:1:547:U:H3      | 1.54                     | 0.55              |
| 1:1:683:G:OP2      | 14:t:35:ARG:NH1   | 2.40                     | 0.55              |
| 1:1:2234:A:C8      | 46:B:1744:G:H4'   | 2.41                     | 0.55              |
| 1:1:2428:G:H22     | 1:1:2475:U:H3     | 1.55                     | 0.55              |
| 1:1:3256:G:H2'     | 1:1:3257:A:H8     | 1.72                     | 0.55              |
| 78:h:174:MET:HB3   | 78:h:181:GLN:HB3  | 1.88                     | 0.55              |
| 1:AS:1156:C:O2     | 33:BZ:46:ARG:NH1  | 2.39                     | 0.55              |
| 1:AS:1655:U:H2'    | 1:AS:1656:C:C6    | 2.41                     | 0.55              |
| 9:BB:19:LYS:HE3    | 9:BB:23:GLU:OE2   | 2.06                     | 0.55              |
| 14:BG:198:GLU:O    | 14:BG:201:LYS:N   | 2.31                     | 0.55              |
| 46:CM:17:C:H2'     | 46:CM:18:C:C6     | 2.41                     | 0.55              |
| 46:CM:72:A:H2'     | 46:CM:73:U:C4'    | 2.36                     | 0.55              |
| 46:CM:1393:U:H2'   | 46:CM:1394:G:C8   | 2.41                     | 0.55              |
| 54:CU:109:PRO:HG2  | 54:CU:112:ARG:HD3 | 1.89                     | 0.55              |
| 54:CU:122:LEU:HD11 | 54:CU:169:TYR:CE1 | 2.42                     | 0.55              |
| 56:CW:68:LYS:HE3   | 56:CW:72:GLU:HG3  | 1.88                     | 0.55              |
| 62:DC:15:PHE:HE2   | 62:DC:17:PHE:HB2  | 1.71                     | 0.55              |
| 62:DC:55:GLY:HA2   | 62:DC:58:LYS:HE2  | 1.89                     | 0.55              |
| 62:DC:77:LYS:HE3   | 62:DC:102:PHE:CE2 | 2.41                     | 0.55              |
| 1:1:1561:U:H2'     | 1:1:1562:G:C8     | 2.40                     | 0.55              |
| 1:1:1795:A:H2'     | 1:1:1796:A:H8     | 1.70                     | 0.55              |
| 7:m:153:THR:HG22   | 7:m:179:ARG:HE    | 1.71                     | 0.55              |
| 7:m:187:ALA:O      | 7:m:189:GLU:N     | 2.39                     | 0.55              |
| 21:0:161:LYS:HB3   | 21:0:161:LYS:NZ   | 2.20                     | 0.55              |
| 23:5:30:GLN:NE2    | 23:5:58:ALA:HB1   | 2.21                     | 0.55              |
| 31:AD:59:GLU:OE1   | 31:AD:71:TYR:OH   | 2.20                     | 0.55              |
| 46:B:370:G:HO2'    | 46:B:609:U:H3     | 1.54                     | 0.55              |
| 46:B:649:G:H3'     | 46:B:650:G:C8     | 2.41                     | 0.55              |
| 46:B:761:G:O6      | 71:a:11:LYS:HE2   | 2.07                     | 0.55              |
| 46:B:1160:U:H2'    | 46:B:1161:G:C8    | 2.41                     | 0.55              |
| 61:Q:119:ASP:O     | 61:Q:120:SER:OG   | 2.20                     | 0.55              |
| 1:AS:116:U:OP1     | 10:BC:142:SER:OG  | 2.24                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AS:925:A:H1'     | 38:CE:49:TRP:CE3  | 2.41                     | 0.55              |
| 1:AS:1539:G:O2'    | 1:AS:2146:A:O2'   | 2.20                     | 0.55              |
| 1:AS:2880:G:O2'    | 41:CH:38:LYS:NZ   | 2.37                     | 0.55              |
| 6:AY:10:ILE:O      | 6:AY:153:VAL:HA   | 2.07                     | 0.55              |
| 46:CM:618:A:N3     | 46:CM:1092:G:O2'  | 2.36                     | 0.55              |
| 46:CM:1774:C:H2'   | 46:CM:1775:G:C8   | 2.42                     | 0.55              |
| 47:CN:180:GLU:OE2  | 47:CN:191:ARG:NH2 | 2.39                     | 0.55              |
| 47:CN:205:ARG:NH2  | 64:DE:82:ASP:OD1  | 2.37                     | 0.55              |
| 48:CO:88:VAL:HG21  | 48:CO:96:LEU:HB3  | 1.88                     | 0.55              |
| 49:CP:134:ILE:HD13 | 49:CP:186:ALA:HB1 | 1.88                     | 0.55              |
| 79:DT:79:ALA:C     | 79:DT:95:LEU:HD23 | 2.32                     | 0.55              |
| 79:DT:258:LYS:HB3  | 79:DT:260:PHE:CZ  | 2.42                     | 0.55              |
| 1:1:40:G:N2        | 1:1:2775:A:N7     | 2.54                     | 0.55              |
| 1:1:2347:G:H2'     | 1:1:2348:G:C8     | 2.41                     | 0.55              |
| 1:1:2583:U:H2'     | 1:1:2584:U:C6     | 2.42                     | 0.55              |
| 1:1:2668:A:N7      | 1:1:2730:A:N6     | 2.55                     | 0.55              |
| 18:x:169:ASN:H     | 18:x:172:GLN:HB2  | 1.71                     | 0.55              |
| 21:0:96:ASP:OD1    | 21:0:97:VAL:N     | 2.40                     | 0.55              |
| 46:B:684:C:H2'     | 46:B:685:C:C6     | 2.41                     | 0.55              |
| 46:B:1265:C:H2'    | 46:B:1266:G:C8    | 2.42                     | 0.55              |
| 46:B:1275:U:H2'    | 46:B:1276:G:C8    | 2.42                     | 0.55              |
| 46:B:1739:U:H2'    | 46:B:1740:A:H8    | 1.71                     | 0.55              |
| 1:AS:705:U:OP2     | 19:BL:168:LYS:NZ  | 2.37                     | 0.55              |
| 1:AS:782:A:H4'     | 1:AS:783:G:H5'    | 1.87                     | 0.55              |
| 1:AS:945:C:O2'     | 1:AS:967:G:OP1    | 2.24                     | 0.55              |
| 1:AS:1695:A:H4'    | 39:CF:3:ARG:NH1   | 2.22                     | 0.55              |
| 1:AS:1903:C:O2     | 5:AX:240:ARG:NH2  | 2.38                     | 0.55              |
| 3:AU:42:G:H1       | 3:AU:102:U:H3     | 1.52                     | 0.55              |
| 8:BA:65:SER:HB3    | 8:BA:75:LEU:HD23  | 1.88                     | 0.55              |
| 9:BB:87:ILE:HD11   | 9:BB:226:THR:HG22 | 1.88                     | 0.55              |
| 31:BX:55:LYS:O     | 31:BX:59:GLU:HG2  | 2.06                     | 0.55              |
| 44:CK:28:LYS:O     | 44:CK:32:GLN:HG3  | 2.07                     | 0.55              |
| 45:CL:156:ALA:HB2  | 57:CX:86:ILE:HB   | 1.88                     | 0.55              |
| 46:CM:108:A:H2'    | 46:CM:109:G:C8    | 2.41                     | 0.55              |
| 46:CM:217:A:H2'    | 46:CM:218:A:O4'   | 2.06                     | 0.55              |
| 46:CM:676:G:OP1    | 46:CM:676:G:H4'   | 2.07                     | 0.55              |
| 46:CM:1066:A:O2'   | 46:CM:1068:G:N7   | 2.39                     | 0.55              |
| 46:CM:1193:A:H4'   | 46:CM:1255:G:P    | 2.46                     | 0.55              |
| 62:DC:81:ARG:NH2   | 62:DC:120:SER:O   | 2.34                     | 0.55              |
| 79:DT:41:THR:HG22  | 79:DT:42:LEU:N    | 2.22                     | 0.55              |
| 81:P0:18:LEU:HA    | 81:P0:21:GLU:HG3  | 1.87                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:139:U:H2'      | 1:1:140:C:C6       | 2.41                     | 0.55              |
| 1:1:1655:U:H3      | 1:1:1786:G:H1      | 1.55                     | 0.55              |
| 31:AD:45:ILE:HD12  | 31:AD:92:LEU:HD11  | 1.89                     | 0.55              |
| 46:B:222:C:H41     | 46:B:823:G:H21     | 1.53                     | 0.55              |
| 46:B:747:A:OP1     | 56:L:79:ARG:NH2    | 2.36                     | 0.55              |
| 46:B:1431:G:N7     | 78:h:131:LYS:NZ    | 2.54                     | 0.55              |
| 54:J:92:ARG:NH1    | 54:J:120:LYS:HB3   | 2.21                     | 0.55              |
| 1:AS:236:A:P       | 3:AU:95:G:H22      | 2.30                     | 0.55              |
| 1:AS:2855:U:H2'    | 1:AS:2856:C:C6     | 2.41                     | 0.55              |
| 3:AU:9:A:H2'       | 3:AU:10:A:C8       | 2.42                     | 0.55              |
| 10:BC:117:ILE:HG12 | 10:BC:123:ALA:CB   | 2.36                     | 0.55              |
| 11:BD:30:PRO:HD2   | 11:BD:82:VAL:O     | 2.06                     | 0.55              |
| 28:BU:13:VAL:HA    | 28:BU:80:LEU:HD23  | 1.89                     | 0.55              |
| 46:CM:638:U:OP1    | 54:CU:97:LYS:NZ    | 2.39                     | 0.55              |
| 46:CM:1516:C:H2'   | 46:CM:1517:C:C6    | 2.42                     | 0.55              |
| 46:CM:1582:U:H5'   | 46:CM:1583:C:OP2   | 2.06                     | 0.55              |
| 48:CO:100:PHE:CD2  | 48:CO:181:LEU:HD11 | 2.40                     | 0.55              |
| 1:1:258:U:H2'      | 1:1:259:C:C6       | 2.42                     | 0.55              |
| 1:1:662:U:H5'      | 6:l:108:ARG:HA     | 1.87                     | 0.55              |
| 1:1:2251:G:H22     | 1:1:2290:A:P       | 2.29                     | 0.55              |
| 9:o:185:GLU:HG2    | 9:o:196:VAL:HG21   | 1.88                     | 0.55              |
| 46:B:1475:U:O2'    | 46:B:1501:A:N6     | 2.37                     | 0.55              |
| 46:B:1712:U:H2'    | 46:B:1713:G:C8     | 2.42                     | 0.55              |
| 50:F:9:LYS:HB3     | 67:W:62:LEU:HD21   | 1.89                     | 0.55              |
| 53:I:69:HIS:HD2    | 53:I:73:VAL:HG11   | 1.71                     | 0.55              |
| 1:AS:523:G:H1      | 1:AS:563:U:H3      | 1.55                     | 0.55              |
| 1:AS:730:A:H2'     | 1:AS:731:U:H2'     | 1.88                     | 0.55              |
| 1:AS:2331:G:H5''   | 18:BK:86:LYS:HB2   | 1.87                     | 0.55              |
| 1:AS:2335:A:H2'    | 1:AS:2336:A:H8     | 1.70                     | 0.55              |
| 1:AS:2376:A:OP1    | 1:AS:2845:U:H4'    | 2.06                     | 0.55              |
| 10:BC:145:GLU:HG2  | 37:CD:38:PHE:HE2   | 1.72                     | 0.55              |
| 23:BP:84:LYS:HD3   | 23:BP:93:ARG:NH2   | 2.21                     | 0.55              |
| 28:BU:57:MET:CG    | 28:BU:61:LYS:HE2   | 2.37                     | 0.55              |
| 37:CD:33:SER:O     | 37:CD:37:VAL:HG23  | 2.06                     | 0.55              |
| 46:CM:78:A:H2'     | 46:CM:79:C:H6      | 1.71                     | 0.55              |
| 46:CM:415:A:H4'    | 46:CM:416:G:O5'    | 2.07                     | 0.55              |
| 46:CM:656:C:H2'    | 46:CM:657:C:C6     | 2.42                     | 0.55              |
| 46:CM:1527:G:OP2   | 65:DF:40:ARG:NH2   | 2.40                     | 0.55              |
| 54:CU:57:PHE:HD2   | 54:CU:91:GLU:HB2   | 1.70                     | 0.55              |
| 66:DG:105:VAL:HB   | 66:DG:122:ARG:HD3  | 1.88                     | 0.55              |
| 1:1:1265:U:H5'     | 1:1:1266:A:OP2     | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:1592:C:O2'     | 1:1:1692:A:N3      | 2.30                     | 0.55              |
| 1:1:2335:A:H2'     | 1:1:2336:A:H8      | 1.72                     | 0.55              |
| 1:1:2527:G:N2      | 1:1:2527:G:OP2     | 2.40                     | 0.55              |
| 1:1:2736:C:N4      | 83:1:3401:3K5:O    | 2.37                     | 0.55              |
| 1:1:2832:U:O2      | 1:1:2910:G:H4'     | 2.06                     | 0.55              |
| 6:l:65:SER:HA      | 6:l:76:PRO:HA      | 1.88                     | 0.55              |
| 14:t:7:LEU:O       | 29:AB:49:HIS:NE2   | 2.39                     | 0.55              |
| 46:B:1354:U:C2     | 46:B:1355:A:N7     | 2.74                     | 0.55              |
| 46:B:1469:A:N3     | 46:B:1594:G:O2'    | 2.29                     | 0.55              |
| 46:B:1637:U:H2'    | 46:B:1638:A:C8     | 2.42                     | 0.55              |
| 1:AS:659:G:P       | 29:BV:12:ARG:HH22  | 2.29                     | 0.55              |
| 1:AS:2899:C:H2'    | 1:AS:2900:C:C6     | 2.40                     | 0.55              |
| 10:BC:43:PRO:HD2   | 10:BC:45:ARG:NH2   | 2.21                     | 0.55              |
| 46:CM:63:G:O2'     | 46:CM:168:U:OP1    | 2.25                     | 0.55              |
| 46:CM:1479:A:H4'   | 46:CM:1480:G:O5'   | 2.07                     | 0.55              |
| 46:CM:1518:G:N2    | 66:DG:48:GLN:OE1   | 2.40                     | 0.55              |
| 52:CS:162:VAL:HG12 | 52:CS:167:ARG:HG3  | 1.89                     | 0.55              |
| 54:CU:63:LEU:HD11  | 54:CU:67:ARG:NH2   | 2.22                     | 0.55              |
| 79:DT:243:SER:HB2  | 79:DT:291:TRP:CE2  | 2.41                     | 0.55              |
| 1:1:357:A:O4'      | 6:l:82:GLY:HA3     | 2.07                     | 0.55              |
| 1:1:1255:A:N7      | 81:P0:53:MET:HB2   | 2.22                     | 0.55              |
| 8:n:104:TYR:OH     | 8:n:134:ARG:HA     | 2.07                     | 0.55              |
| 11:q:10:LEU:HD21   | 11:q:79:ILE:HD11   | 1.88                     | 0.55              |
| 41:AN:3:GLU:HG3    | 41:AN:6:LEU:H      | 1.72                     | 0.55              |
| 46:B:821:U:H2'     | 46:B:822:G:C8      | 2.41                     | 0.55              |
| 46:B:1240:G:N7     | 59:O:46:ARG:NH2    | 2.48                     | 0.55              |
| 1:AS:795:G:O2'     | 14:BG:18:TRP:CD1   | 2.59                     | 0.55              |
| 1:AS:3317:U:O2'    | 55:CV:168:SER:HB2  | 2.06                     | 0.55              |
| 26:BS:24:LEU:HD23  | 26:BS:25:LYS:N     | 2.22                     | 0.55              |
| 48:CO:30:PHE:HE2   | 48:CO:48:ILE:HG22  | 1.72                     | 0.55              |
| 48:CO:223:PHE:HZ   | 48:CO:228:LEU:HD13 | 1.71                     | 0.55              |
| 52:CS:76:LYS:HG2   | 63:DD:121:ARG:CZ   | 2.36                     | 0.55              |
| 52:CS:110:ALA:O    | 52:CS:114:VAL:HG23 | 2.07                     | 0.55              |
| 65:DF:15:LEU:HB2   | 65:DF:22:ILE:HB    | 1.88                     | 0.55              |
| 79:DT:88:ARG:NH2   | 79:DT:108:LYS:O    | 2.39                     | 0.55              |
| 79:DT:150:ASP:N    | 79:DT:172:ASP:HB3  | 2.21                     | 0.55              |
| 1:1:248:U:H2'      | 1:1:249:G:H4'      | 1.89                     | 0.54              |
| 1:1:788:G:H2'      | 1:1:789:C:C6       | 2.43                     | 0.54              |
| 1:1:2584:U:H2'     | 1:1:2585:U:O4'     | 2.07                     | 0.54              |
| 1:1:2855:U:H2'     | 1:1:2856:C:H6      | 1.72                     | 0.54              |
| 1:1:3166:A:H2'     | 1:1:3167:G:H8      | 1.72                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:O:42:TRP:O     | 21:O:46:GLN:HG3    | 2.08                     | 0.54              |
| 30:AC:58:ARG:HG3  | 30:AC:59:ALA:H     | 1.70                     | 0.54              |
| 46:B:227:C:H2'    | 46:B:228:C:O4'     | 2.07                     | 0.54              |
| 46:B:334:G:O6     | 55:K:5:ARG:NH1     | 2.39                     | 0.54              |
| 46:B:446:C:OP1    | 51:G:29:PRO:HD3    | 2.07                     | 0.54              |
| 46:B:1067:C:H4'   | 68:X:58:TYR:CE2    | 2.43                     | 0.54              |
| 64:T:89:SER:C     | 64:T:91:LEU:H      | 2.15                     | 0.54              |
| 1:AS:187:U:O2'    | 1:AS:206:U:O2      | 2.24                     | 0.54              |
| 1:AS:1007:A:H2'   | 1:AS:1008:A:H8     | 1.72                     | 0.54              |
| 1:AS:1014:G:H2'   | 1:AS:1015:G:H8     | 1.71                     | 0.54              |
| 1:AS:2244:U:H2'   | 1:AS:2245:C:C6     | 2.42                     | 0.54              |
| 1:AS:2384:C:H2'   | 1:AS:2385:C:C6     | 2.42                     | 0.54              |
| 4:AW:96:LEU:O     | 44:CK:87:ARG:HD3   | 2.08                     | 0.54              |
| 5:AX:117:ARG:HD2  | 5:AX:176:ALA:O     | 2.06                     | 0.54              |
| 11:BD:47:LYS:HE3  | 11:BD:49:ASN:O     | 2.07                     | 0.54              |
| 14:BG:195:ALA:O   | 14:BG:199:LYS:CB   | 2.55                     | 0.54              |
| 26:BS:70:GLU:HG2  | 26:BS:74:LYS:HZ2   | 1.72                     | 0.54              |
| 51:CR:100:ARG:HG2 | 51:CR:102:VAL:HG13 | 1.89                     | 0.54              |
| 79:DT:67:HIS:ND1  | 79:DT:86:TRP:HB2   | 2.22                     | 0.54              |
| 1:1:362:U:O4      | 38:AK:24:ARG:NH2   | 2.40                     | 0.54              |
| 1:1:1791:U:H2'    | 4:j:50:HIS:CD2     | 2.43                     | 0.54              |
| 14:t:155:GLU:OE2  | 14:t:159:ARG:NE    | 2.40                     | 0.54              |
| 19:y:54:LEU:HD22  | 19:y:58:ASN:HB3    | 1.89                     | 0.54              |
| 25:7:80:ARG:NH2   | 46:B:163:G:O2'     | 2.39                     | 0.54              |
| 45:i:104:GLN:HA   | 45:i:109:GLN:NE2   | 2.22                     | 0.54              |
| 46:B:327:G:H5''   | 55:K:98:LYS:HB3    | 1.88                     | 0.54              |
| 46:B:1600:U:OP1   | 52:H:169:ASN:HB2   | 2.06                     | 0.54              |
| 1:AS:411:U:H2'    | 1:AS:412:G:H8      | 1.71                     | 0.54              |
| 1:AS:1110:U:OP1   | 29:BV:23:GLY:N     | 2.29                     | 0.54              |
| 1:AS:1184:U:OP1   | 1:AS:1206:U:O2'    | 2.17                     | 0.54              |
| 2:AT:3:U:H2'      | 2:AT:4:U:H6        | 1.72                     | 0.54              |
| 7:AZ:178:ASN:HA   | 7:AZ:183:TRP:CD2   | 2.42                     | 0.54              |
| 10:BC:50:PHE:O    | 26:BS:30:THR:HG22  | 2.07                     | 0.54              |
| 11:BD:16:VAL:HG11 | 11:BD:79:ILE:HG13  | 1.90                     | 0.54              |
| 23:BP:19:VAL:HG13 | 23:BP:22:PRO:HG2   | 1.88                     | 0.54              |
| 46:CM:4:C:H5      | 46:CM:20:G:H1      | 1.56                     | 0.54              |
| 46:CM:638:U:H2'   | 46:CM:639:G:O4'    | 2.06                     | 0.54              |
| 46:CM:1602:C:P    | 52:CS:81:ARG:HE    | 2.30                     | 0.54              |
| 52:CS:125:THR:O   | 52:CS:127:GLN:HG3  | 2.07                     | 0.54              |
| 62:DC:30:THR:O    | 62:DC:34:THR:HG23  | 2.07                     | 0.54              |
| 79:DT:34:LEU:HB3  | 79:DT:74:ILE:HD11  | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 82:12:151:ILE:O    | 82:12:155:ILE:HG12 | 2.07                     | 0.54              |
| 1:1:1442:A:H61     | 1:1:2334:A:H5''    | 1.72                     | 0.54              |
| 1:1:1655:U:H2'     | 1:1:1656:C:C6      | 2.42                     | 0.54              |
| 1:1:2587:G:H2'     | 1:1:2588:C:C6      | 2.41                     | 0.54              |
| 29:AB:76:ASP:OD1   | 29:AB:76:ASP:N     | 2.40                     | 0.54              |
| 45:i:132:GLU:HG2   | 50:F:91:ARG:HH22   | 1.73                     | 0.54              |
| 46:B:405:A:H2'     | 46:B:406:C:C6      | 2.43                     | 0.54              |
| 46:B:536:A:H1'     | 46:B:539:A:C8      | 2.43                     | 0.54              |
| 49:E:163:ARG:HD3   | 49:E:165:ILE:HD11  | 1.88                     | 0.54              |
| 50:F:68:HIS:CE1    | 57:M:94:ASN:HB3    | 2.42                     | 0.54              |
| 64:T:71:PHE:CZ     | 64:T:74:GLN:HB2    | 2.43                     | 0.54              |
| 1:AS:1011:C:N4     | 1:AS:1031:A:H61    | 2.05                     | 0.54              |
| 14:BG:59:ARG:HH22  | 14:BG:152:PRO:HG2  | 1.72                     | 0.54              |
| 36:CC:4:VAL:HG12   | 36:CC:53:ARG:HH11  | 1.72                     | 0.54              |
| 46:CM:585:C:H5''   | 77:DR:26:LYS:HZ1   | 1.72                     | 0.54              |
| 46:CM:970:G:H2'    | 46:CM:971:G:H8     | 1.71                     | 0.54              |
| 46:CM:1140:G:H2'   | 46:CM:1141:C:C6    | 2.42                     | 0.54              |
| 54:CU:68:LYS:O     | 54:CU:72:ARG:NE    | 2.37                     | 0.54              |
| 55:CV:84:HIS:NE2   | 55:CV:97:THR:OG1   | 2.29                     | 0.54              |
| 59:CZ:71:ILE:HA    | 59:CZ:74:LEU:HB2   | 1.89                     | 0.54              |
| 1:1:2385:C:H2'     | 1:1:2386:U:H6      | 1.73                     | 0.54              |
| 1:1:3138:U:H2'     | 1:1:3139:U:C6      | 2.42                     | 0.54              |
| 16:v:183:THR:HG22  | 16:v:187:ARG:HB2   | 1.88                     | 0.54              |
| 46:B:728:U:P       | 54:J:104:LYS:H     | 2.30                     | 0.54              |
| 46:B:845:U:O4'     | 54:J:110:ARG:HG3   | 2.07                     | 0.54              |
| 47:C:84:ARG:NE     | 64:T:82:ASP:OD1    | 2.35                     | 0.54              |
| 49:E:97:VAL:HG11   | 49:E:124:ILE:HG12  | 1.89                     | 0.54              |
| 50:F:116:ILE:HG13  | 50:F:117:ARG:N     | 2.21                     | 0.54              |
| 77:g:55:LYS:HB2    | 77:g:58:PRO:HG3    | 1.89                     | 0.54              |
| 1:AS:429:U:H2'     | 1:AS:430:G:C8      | 2.37                     | 0.54              |
| 1:AS:498:C:H2'     | 1:AS:499:G:H8      | 1.73                     | 0.54              |
| 1:AS:1434:U:H4'    | 6:AY:89:ALA:HB3    | 1.89                     | 0.54              |
| 1:AS:2689:U:H3     | 1:AS:2711:A:H2     | 1.54                     | 0.54              |
| 1:AS:2873:G:O2'    | 1:AS:2996:A:N1     | 2.39                     | 0.54              |
| 6:AY:262:VAL:HA    | 6:AY:271:ILE:HG12  | 1.89                     | 0.54              |
| 8:BA:55:LYS:NZ     | 8:BA:97:VAL:O      | 2.30                     | 0.54              |
| 13:BF:106:ILE:HD11 | 13:BF:125:MET:HB3  | 1.88                     | 0.54              |
| 21:BN:52:LYS:HG2   | 21:BN:55:SER:HB3   | 1.89                     | 0.54              |
| 46:CM:213:A:N7     | 46:CM:240:U:H2'    | 2.22                     | 0.54              |
| 46:CM:623:C:H2'    | 46:CM:624:U:C6     | 2.43                     | 0.54              |
| 46:CM:897:U:OP1    | 46:CM:898:G:O2'    | 2.19                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1776:G:OP1   | 73:DN:17:HIS:NE2   | 2.35                     | 0.54              |
| 48:CO:83:LYS:O     | 48:CO:103:LEU:HD12 | 2.08                     | 0.54              |
| 59:CZ:42:ALA:HB1   | 59:CZ:47:GLU:C     | 2.32                     | 0.54              |
| 59:CZ:62:LEU:HD12  | 59:CZ:63:CYS:O     | 2.06                     | 0.54              |
| 79:DT:135:TRP:CZ2  | 79:DT:141:CYS:HB2  | 2.42                     | 0.54              |
| 1:1:623:A:H2'      | 1:1:624:U:C6       | 2.43                     | 0.54              |
| 1:1:948:A:H4'      | 1:1:964:G:N2       | 2.23                     | 0.54              |
| 1:1:1094:A:OP2     | 22:2:130:ARG:NE    | 2.25                     | 0.54              |
| 1:1:2666:A:H2'     | 1:1:2667:A:C8      | 2.42                     | 0.54              |
| 3:4:126:A:O2'      | 3:4:129:C:N4       | 2.41                     | 0.54              |
| 45:i:114:GLU:HG2   | 45:i:115:LEU:N     | 2.22                     | 0.54              |
| 46:B:142:G:O2'     | 46:B:143:A:O5'     | 2.19                     | 0.54              |
| 1:AS:146:U:OP1     | 10:BC:196:SER:HA   | 2.07                     | 0.54              |
| 1:AS:583:A:H2'     | 1:AS:584:C:C6      | 2.42                     | 0.54              |
| 1:AS:783:G:H2'     | 1:AS:784:C:C6      | 2.43                     | 0.54              |
| 1:AS:1611:U:H2'    | 1:AS:1612:U:H6     | 1.72                     | 0.54              |
| 1:AS:2234:A:N7     | 46:CM:1744:G:H5'   | 2.22                     | 0.54              |
| 1:AS:2391:A:H2'    | 1:AS:2392:G:H8     | 1.72                     | 0.54              |
| 39:CF:72:THR:OG1   | 39:CF:73:LEU:HD12  | 2.07                     | 0.54              |
| 40:CG:44:TRP:O     | 40:CG:48:LYS:NZ    | 2.32                     | 0.54              |
| 46:CM:338:U:H2'    | 46:CM:339:A:H8     | 1.72                     | 0.54              |
| 46:CM:872:A:H5''   | 61:DB:115:PRO:HB2  | 1.90                     | 0.54              |
| 46:CM:1245:U:H2'   | 46:CM:1246:G:H8    | 1.73                     | 0.54              |
| 47:CN:84:ARG:HD3   | 47:CN:203:PHE:O    | 2.08                     | 0.54              |
| 59:CZ:102:GLY:C    | 59:CZ:104:CYS:N    | 2.62                     | 0.54              |
| 79:DT:69:VAL:HA    | 79:DT:85:SER:HA    | 1.88                     | 0.54              |
| 79:DT:277:VAL:HG13 | 79:DT:278:GLY:N    | 2.21                     | 0.54              |
| 81:P0:30:VAL:HB    | 81:P0:33:VAL:HG21  | 1.90                     | 0.54              |
| 1:1:698:C:H2'      | 1:1:699:G:H8       | 1.73                     | 0.54              |
| 1:1:1115:C:H2'     | 1:1:1116:A:C8      | 2.43                     | 0.54              |
| 1:1:2520:A:H1'     | 1:1:2521:C:C5      | 2.43                     | 0.54              |
| 46:B:108:A:H2'     | 46:B:109:G:C8      | 2.43                     | 0.54              |
| 46:B:626:G:N1      | 46:B:955:A:OP2     | 2.32                     | 0.54              |
| 46:B:880:G:H1      | 46:B:902:U:H3      | 1.55                     | 0.54              |
| 51:G:151:ASP:HB3   | 51:G:154:ILE:HG13  | 1.90                     | 0.54              |
| 1:AS:795:G:O2'     | 14:BG:18:TRP:NE1   | 2.40                     | 0.54              |
| 1:AS:1218:G:H4'    | 1:AS:1219:A:H5''   | 1.90                     | 0.54              |
| 1:AS:1417:G:H2'    | 1:AS:1418:G:H8     | 1.71                     | 0.54              |
| 1:AS:2107:U:H2'    | 1:AS:2108:G:C8     | 2.42                     | 0.54              |
| 20:BM:175:GLN:O    | 20:BM:179:GLU:HG3  | 2.07                     | 0.54              |
| 29:BV:126:LYS:HE2  | 29:BV:148:VAL:HG11 | 1.90                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:CC:85:THR:O    | 36:CC:89:ARG:HG3   | 2.08                     | 0.54              |
| 46:CM:151:G:H2'   | 46:CM:152:G:C8     | 2.43                     | 0.54              |
| 46:CM:585:C:H5'   | 77:DR:24:GLN:OE1   | 2.08                     | 0.54              |
| 79:DT:219:LEU:HG  | 79:DT:229:TYR:CZ   | 2.43                     | 0.54              |
| 82:12:116:MET:O   | 82:12:119:LYS:HG2  | 2.07                     | 0.54              |
| 1:1:92:C:OP2      | 1:1:2736:C:O2'     | 2.21                     | 0.54              |
| 1:1:619:A:O2'     | 34:AG:60:ARG:NH2   | 2.40                     | 0.54              |
| 1:1:1661:U:H2'    | 1:1:1662:G:H8      | 1.73                     | 0.54              |
| 1:1:2158:A:H2'    | 1:1:2159:C:C6      | 2.43                     | 0.54              |
| 1:1:2477:U:H2'    | 1:1:2478:A:H8      | 1.73                     | 0.54              |
| 8:n:95:VAL:HG22   | 8:n:144:ALA:HB3    | 1.89                     | 0.54              |
| 46:B:302:U:H2'    | 46:B:303:C:C6      | 2.42                     | 0.54              |
| 46:B:786:G:H2'    | 46:B:787:A:C8      | 2.43                     | 0.54              |
| 46:B:875:C:H2'    | 46:B:876:A:H8      | 1.73                     | 0.54              |
| 50:F:110:LEU:HD21 | 50:F:116:ILE:HG22  | 1.89                     | 0.54              |
| 64:T:72:LYS:NZ    | 64:T:76:GLU:OE2    | 2.38                     | 0.54              |
| 1:AS:364:G:OP1    | 6:AY:61:THR:HG23   | 2.07                     | 0.54              |
| 1:AS:662:U:H2'    | 1:AS:663:A:H8      | 1.72                     | 0.54              |
| 1:AS:2418:A:H2'   | 1:AS:2419:A:C8     | 2.42                     | 0.54              |
| 1:AS:3133:G:H2'   | 1:AS:3134:C:O4'    | 2.08                     | 0.54              |
| 21:BN:44:PHE:HE1  | 21:BN:122:HIS:ND1  | 2.06                     | 0.54              |
| 26:BS:47:GLN:NE2  | 26:BS:49:LYS:HG2   | 2.23                     | 0.54              |
| 46:CM:446:C:OP1   | 51:CR:29:PRO:HD3   | 2.08                     | 0.54              |
| 46:CM:768:C:H2'   | 46:CM:769:U:O4'    | 2.07                     | 0.54              |
| 46:CM:886:G:H2'   | 46:CM:887:G:C8     | 2.42                     | 0.54              |
| 48:CO:36:THR:HG23 | 48:CO:232:HIS:HA   | 1.88                     | 0.54              |
| 48:CO:216:LYS:HD2 | 48:CO:218:LEU:CD2  | 2.37                     | 0.54              |
| 51:CR:182:MET:HB2 | 51:CR:228:ILE:HD13 | 1.89                     | 0.54              |
| 59:CZ:121:VAL:O   | 59:CZ:122:VAL:HG23 | 2.07                     | 0.54              |
| 61:DB:76:ILE:HD13 | 61:DB:97:LEU:HD11  | 1.88                     | 0.54              |
| 77:DR:13:LYS:O    | 77:DR:17:GLN:HG2   | 2.08                     | 0.54              |
| 79:DT:175:VAL:HB  | 79:DT:189:PHE:HB2  | 1.90                     | 0.54              |
| 81:P0:66:PHE:CE2  | 81:P0:69:GLU:HB3   | 2.42                     | 0.54              |
| 81:P0:76:LEU:HA   | 81:P0:79:PHE:HE1   | 1.71                     | 0.54              |
| 1:1:960:G:OP2     | 1:1:1111:G:N1      | 2.41                     | 0.54              |
| 1:1:1035:U:H2'    | 1:1:1036:A:C8      | 2.43                     | 0.54              |
| 1:1:1617:A:H2'    | 1:1:1618:U:C6      | 2.43                     | 0.54              |
| 1:1:2888:U:H5     | 1:1:2907:U:HO2'    | 1.55                     | 0.54              |
| 1:1:3285:A:H2'    | 1:1:3286:C:C6      | 2.42                     | 0.54              |
| 3:4:70:G:H5''     | 27:9:28:ARG:CZ     | 2.37                     | 0.54              |
| 46:B:1:U:HO2'     | 46:B:3:U:H5        | 1.56                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:151:G:H2'    | 46:B:152:G:H8      | 1.71                     | 0.54              |
| 79:AR:16:HIS:CD2  | 79:AR:43:ILE:HD12  | 2.42                     | 0.54              |
| 1:AS:336:A:O2'    | 6:AY:49:GLN:OE1    | 2.19                     | 0.54              |
| 1:AS:1580:U:H2'   | 1:AS:1581:C:C6     | 2.43                     | 0.54              |
| 1:AS:2853:C:H2'   | 1:AS:2854:U:C6     | 2.43                     | 0.54              |
| 14:BG:122:LYS:HD2 | 14:BG:147:PHE:CZ   | 2.42                     | 0.54              |
| 16:BI:73:ARG:NH1  | 16:BI:86:ASN:O     | 2.40                     | 0.54              |
| 16:BI:143:ARG:O   | 16:BI:149:ASN:ND2  | 2.38                     | 0.54              |
| 45:CL:63:ALA:O    | 45:CL:65:LYS:N     | 2.40                     | 0.54              |
| 46:CM:14:C:H2'    | 46:CM:15:U:C6      | 2.43                     | 0.54              |
| 46:CM:472:A:H5''  | 56:CW:144:PRO:HD2  | 1.90                     | 0.54              |
| 1:1:431:A:H2'     | 1:1:432:G:C8       | 2.42                     | 0.54              |
| 1:1:2130:A:H2'    | 1:1:2131:U:H6      | 1.73                     | 0.54              |
| 1:1:2234:A:N7     | 46:B:1744:G:H4'    | 2.23                     | 0.54              |
| 1:1:2959:A:H2'    | 1:1:2960:C:H6      | 1.73                     | 0.54              |
| 1:1:3216:U:H2'    | 1:1:3217:G:C8      | 2.42                     | 0.54              |
| 46:B:753:C:C2     | 56:L:143:ILE:HG21  | 2.42                     | 0.54              |
| 46:B:820:U:OP1    | 46:B:820:U:H4'     | 2.07                     | 0.54              |
| 46:B:1323:C:H1'   | 46:B:1396:A:C5     | 2.43                     | 0.54              |
| 46:B:1369:G:OP1   | 67:W:86:HIS:ND1    | 2.41                     | 0.54              |
| 46:B:1596:U:H5''  | 63:S:74:VAL:HB     | 1.90                     | 0.54              |
| 1:AS:1380:U:OP2   | 6:AY:203:ARG:HA    | 2.08                     | 0.54              |
| 1:AS:2958:U:H2'   | 1:AS:2959:A:H8     | 1.73                     | 0.54              |
| 5:AX:284:ARG:HH11 | 5:AX:356:LEU:HD12  | 1.73                     | 0.54              |
| 6:AY:113:LYS:HD2  | 16:BI:203:ARG:O    | 2.07                     | 0.54              |
| 8:BA:148:GLU:OE1  | 8:BA:151:LYS:NZ    | 2.40                     | 0.54              |
| 10:BC:136:GLY:O   | 10:BC:140:VAL:HG23 | 2.07                     | 0.54              |
| 11:BD:90:MET:HE3  | 11:BD:181:VAL:HG23 | 1.89                     | 0.54              |
| 18:BK:118:GLN:OE1 | 18:BK:120:ASN:ND2  | 2.39                     | 0.54              |
| 21:BN:8:GLN:HG3   | 21:BN:26:ARG:HD2   | 1.90                     | 0.54              |
| 52:CS:159:ALA:CB  | 52:CS:225:ARG:HG2  | 2.37                     | 0.54              |
| 54:CU:94:ILE:HG21 | 54:CU:114:LEU:HD12 | 1.90                     | 0.54              |
| 54:CU:160:TYR:CE2 | 54:CU:161:LYS:HG2  | 2.43                     | 0.54              |
| 54:CU:169:TYR:CE2 | 54:CU:175:LYS:HB2  | 2.43                     | 0.54              |
| 56:CW:53:ARG:O    | 56:CW:57:ARG:N     | 2.34                     | 0.54              |
| 62:DC:58:LYS:HE3  | 62:DC:59:LYS:HG2   | 1.90                     | 0.54              |
| 75:DP:18:ARG:HD2  | 75:DP:26:THR:HG22  | 1.89                     | 0.54              |
| 81:P0:70:LEU:HB3  | 81:P0:72:GLU:CD    | 2.32                     | 0.54              |
| 1:1:173:C:H2'     | 1:1:174:C:C6       | 2.42                     | 0.54              |
| 1:1:1279:C:H2'    | 1:1:1280:C:H6      | 1.72                     | 0.54              |
| 1:1:2446:A:H1'    | 1:1:2456:C:O2      | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3:112:G:H2'      | 2:3:113:C:C6       | 2.43                     | 0.54              |
| 16:v:62:TYR:HD2    | 16:v:106:VAL:HG13  | 1.72                     | 0.54              |
| 46:B:1470:G:H5'    | 63:S:14:THR:HG21   | 1.88                     | 0.54              |
| 54:J:29:ASP:OD1    | 54:J:30:LEU:HD23   | 2.07                     | 0.54              |
| 64:T:99:GLN:OE1    | 64:T:99:GLN:N      | 2.41                     | 0.54              |
| 79:AR:38:ARG:HA    | 79:AR:68:ILE:HG23  | 1.88                     | 0.54              |
| 79:AR:90:LEU:HD11  | 79:AR:125:SER:HB3  | 1.89                     | 0.54              |
| 1:AS:35:C:H4'      | 1:AS:804:A:C2      | 2.43                     | 0.54              |
| 1:AS:1519:U:H4'    | 26:BS:112:THR:O    | 2.08                     | 0.54              |
| 14:BG:12:ASN:O     | 14:BG:15:ARG:NH1   | 2.40                     | 0.54              |
| 35:CB:103:ARG:O    | 35:CB:107:GLU:OE1  | 2.25                     | 0.54              |
| 46:CM:333:U:O2'    | 58:CY:130:PRO:O    | 2.18                     | 0.54              |
| 46:CM:924:A:H2'    | 46:CM:925:A:C8     | 2.43                     | 0.54              |
| 54:CU:136:VAL:HG22 | 54:CU:146:GLN:HG3  | 1.90                     | 0.54              |
| 64:DE:89:SER:C     | 64:DE:91:LEU:H     | 2.16                     | 0.54              |
| 69:DJ:2:THR:CG2    | 69:DJ:3:ARG:H      | 2.15                     | 0.54              |
| 79:DT:198:CYS:O    | 79:DT:199:ILE:HD13 | 2.08                     | 0.54              |
| 1:1:629:A:C2       | 34:AG:91:PRO:HG2   | 2.43                     | 0.53              |
| 1:1:1014:G:N2      | 1:1:1030:U:O2      | 2.39                     | 0.53              |
| 1:1:2174:C:O2'     | 1:1:2248:A:N3      | 2.37                     | 0.53              |
| 1:1:2431:U:H5'     | 1:1:2439:A:H5'     | 1.90                     | 0.53              |
| 1:1:2958:U:H2'     | 1:1:2959:A:C8      | 2.43                     | 0.53              |
| 1:1:2959:A:H2'     | 1:1:2960:C:C6      | 2.43                     | 0.53              |
| 1:1:3014:U:OP2     | 1:1:3064:C:N4      | 2.31                     | 0.53              |
| 14:t:76:THR:HG22   | 14:t:101:ARG:HB3   | 1.90                     | 0.53              |
| 52:H:91:GLU:HA     | 52:H:94:THR:HG22   | 1.89                     | 0.53              |
| 57:M:15:LEU:O      | 57:M:19:GLY:HA2    | 2.07                     | 0.53              |
| 57:M:70:ASP:OD1    | 57:M:71:GLU:N      | 2.41                     | 0.53              |
| 58:N:19:ILE:HG23   | 58:N:32:LYS:HE2    | 1.90                     | 0.53              |
| 1:AS:498:C:H2'     | 1:AS:499:G:C8      | 2.42                     | 0.53              |
| 1:AS:948:A:H4'     | 1:AS:964:G:N2      | 2.22                     | 0.53              |
| 1:AS:1569:C:H2'    | 1:AS:1570:A:C8     | 2.43                     | 0.53              |
| 1:AS:1618:U:H2'    | 1:AS:1619:G:C8     | 2.43                     | 0.53              |
| 1:AS:2093:G:H22    | 1:AS:2098:A:H1'    | 1.73                     | 0.53              |
| 1:AS:2484:U:H2'    | 1:AS:2485:U:C6     | 2.43                     | 0.53              |
| 1:AS:2871:C:C5     | 11:BD:171:ASP:HA   | 2.43                     | 0.53              |
| 2:AT:3:U:H2'       | 2:AT:4:U:C6        | 2.43                     | 0.53              |
| 32:BY:18:ARG:HB3   | 32:BY:34:GLU:HG3   | 1.90                     | 0.53              |
| 36:CC:34:GLN:O     | 36:CC:38:ARG:N     | 2.41                     | 0.53              |
| 46:CM:652:C:H5'    | 46:CM:653:G:OP2    | 2.07                     | 0.53              |
| 46:CM:1130:U:O2'   | 49:CP:84:GLN:O     | 2.25                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1470:G:H5'   | 63:DD:14:THR:HG21  | 1.90                     | 0.53              |
| 57:CX:78:THR:O     | 57:CX:81:ASN:ND2   | 2.41                     | 0.53              |
| 77:DR:22:GLU:O     | 77:DR:24:GLN:NE2   | 2.42                     | 0.53              |
| 78:DS:167:THR:OG1  | 78:DS:168:CYS:N    | 2.40                     | 0.53              |
| 79:DT:31:ASP:HA    | 79:DT:47:LEU:HB3   | 1.90                     | 0.53              |
| 79:DT:248:TRP:CD1  | 79:DT:261:LYS:HA   | 2.43                     | 0.53              |
| 82:12:125:LEU:HD21 | 82:12:164:GLU:O    | 2.07                     | 0.53              |
| 1:1:374:A:N3       | 1:1:376:G:H5''     | 2.23                     | 0.53              |
| 1:1:612:U:H2'      | 1:1:613:U:C6       | 2.42                     | 0.53              |
| 1:1:619:A:H2'      | 1:1:620:A:C8       | 2.44                     | 0.53              |
| 1:1:2520:A:H1'     | 1:1:2521:C:H5      | 1.74                     | 0.53              |
| 1:1:2836:A:H5''    | 12:r:114:GLY:HA2   | 1.89                     | 0.53              |
| 1:1:3044:C:H2'     | 1:1:3045:A:O4'     | 2.09                     | 0.53              |
| 2:3:97:A:OP1       | 21:0:40:ARG:NH1    | 2.41                     | 0.53              |
| 19:y:123:THR:OG1   | 19:y:125:ASP:OD1   | 2.21                     | 0.53              |
| 51:G:141:THR:OG1   | 51:G:143:ASP:OD1   | 2.22                     | 0.53              |
| 52:H:43:PHE:HE1    | 52:H:70:VAL:HG23   | 1.73                     | 0.53              |
| 52:H:103:ASN:HA    | 52:H:106:LYS:HD2   | 1.91                     | 0.53              |
| 67:W:32:GLN:OE1    | 67:W:32:GLN:N      | 2.41                     | 0.53              |
| 1:AS:412:G:H5'     | 18:BK:26:PHE:HZ    | 1.74                     | 0.53              |
| 1:AS:427:C:OP1     | 33:BZ:14:TYR:OH    | 2.23                     | 0.53              |
| 1:AS:619:A:H2'     | 1:AS:620:A:N7      | 2.22                     | 0.53              |
| 1:AS:2739:U:H2'    | 1:AS:2740:U:C6     | 2.43                     | 0.53              |
| 1:AS:3110:U:OP1    | 5:AX:274:HIS:ND1   | 2.40                     | 0.53              |
| 16:BI:113:LEU:HB2  | 16:BI:134:LEU:HD23 | 1.89                     | 0.53              |
| 46:CM:336:C:H5''   | 55:CV:10:LYS:HD2   | 1.89                     | 0.53              |
| 46:CM:921:G:OP1    | 46:CM:1059:G:N2    | 2.34                     | 0.53              |
| 46:CM:1578:C:H2'   | 46:CM:1579:A:C8    | 2.43                     | 0.53              |
| 49:CP:171:LYS:HE3  | 49:CP:192:TYR:OH   | 2.09                     | 0.53              |
| 52:CS:116:HIS:O    | 52:CS:120:ILE:HG13 | 2.08                     | 0.53              |
| 52:CS:165:LEU:HG   | 52:CS:169:ASN:HD22 | 1.73                     | 0.53              |
| 54:CU:159:ASP:HA   | 54:CU:162:LEU:HD21 | 1.91                     | 0.53              |
| 62:DC:31:GLU:O     | 62:DC:34:THR:OG1   | 2.24                     | 0.53              |
| 64:DE:80:ARG:HA    | 64:DE:83:GLN:NE2   | 2.23                     | 0.53              |
| 81:P0:73:PHE:C     | 81:P0:75:LYS:H     | 2.15                     | 0.53              |
| 1:1:339:C:OP1      | 1:1:1376:G:O2'     | 2.24                     | 0.53              |
| 1:1:1251:C:H2'     | 1:1:1252:G:H8      | 1.73                     | 0.53              |
| 1:1:1863:A:H2'     | 1:1:1864:G:H8      | 1.71                     | 0.53              |
| 1:1:3081:G:N2      | 11:q:156:GLN:OE1   | 2.40                     | 0.53              |
| 1:1:3125:U:H4'     | 1:1:3126:U:O4'     | 2.07                     | 0.53              |
| 7:m:95:TRP:CD1     | 7:m:158:ARG:HA     | 2.43                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:u:19:VAL:HG12   | 15:u:57:LEU:HA     | 1.89                     | 0.53              |
| 21:0:171:PHE:O     | 21:0:172:TYR:HB2   | 2.08                     | 0.53              |
| 46:B:122:U:C2'     | 46:B:123:G:H5''    | 2.37                     | 0.53              |
| 1:AS:666:G:H4'     | 19:BL:164:ARG:HD3  | 1.89                     | 0.53              |
| 1:AS:730:A:H4'     | 1:AS:730:A:OP1     | 2.08                     | 0.53              |
| 1:AS:2116:A:C4     | 38:CE:3:LYS:HB3    | 2.42                     | 0.53              |
| 2:AT:112:G:H2'     | 2:AT:113:C:C6      | 2.43                     | 0.53              |
| 24:BQ:30:GLY:HA3   | 24:BQ:66:LYS:HE2   | 1.91                     | 0.53              |
| 46:CM:86:A:H5'     | 71:DL:119:PHE:CE1  | 2.44                     | 0.53              |
| 46:CM:138:C:O4'    | 53:CT:179:VAL:HG11 | 2.08                     | 0.53              |
| 46:CM:1029:U:H2'   | 46:CM:1030:C:C6    | 2.43                     | 0.53              |
| 50:CQ:133:LYS:HB3  | 50:CQ:190:MET:HE2  | 1.90                     | 0.53              |
| 79:DT:70:GLN:N     | 79:DT:84:ALA:O     | 2.37                     | 0.53              |
| 1:1:631:U:H2'      | 1:1:632:C:C6       | 2.44                     | 0.53              |
| 1:1:787:A:H2'      | 1:1:788:G:H8       | 1.73                     | 0.53              |
| 1:1:1762:G:O2'     | 1:1:1763:C:OP1     | 2.25                     | 0.53              |
| 1:1:2639:A:N6      | 1:1:2659:G:O2'     | 2.41                     | 0.53              |
| 27:9:45:VAL:HG12   | 27:9:46:LYS:N      | 2.20                     | 0.53              |
| 31:AD:12:ILE:HD12  | 31:AD:15:LYS:HD2   | 1.89                     | 0.53              |
| 46:B:78:A:H2'      | 46:B:79:C:C6       | 2.43                     | 0.53              |
| 47:C:52:LYS:HD3    | 68:X:82:VAL:HG23   | 1.91                     | 0.53              |
| 1:AS:299:G:C8      | 37:CD:30:GLY:HA3   | 2.43                     | 0.53              |
| 1:AS:607:G:OP2     | 6:AY:316:LYS:NZ    | 2.41                     | 0.53              |
| 1:AS:1593:C:H2'    | 1:AS:1594:G:H8     | 1.73                     | 0.53              |
| 1:AS:1618:U:H2'    | 1:AS:1619:G:H8     | 1.73                     | 0.53              |
| 14:BG:80:LEU:HD11  | 14:BG:97:VAL:HG22  | 1.91                     | 0.53              |
| 19:BL:79:LYS:HE3   | 19:BL:138:LEU:HD12 | 1.89                     | 0.53              |
| 20:BM:70:LYS:HB3   | 20:BM:76:MET:HE2   | 1.90                     | 0.53              |
| 28:BU:46:ILE:HD12  | 28:BU:130:PHE:O    | 2.09                     | 0.53              |
| 28:BU:117:ALA:O    | 28:BU:121:LYS:HG2  | 2.08                     | 0.53              |
| 46:CM:1495:U:H2'   | 46:CM:1496:C:C6    | 2.44                     | 0.53              |
| 46:CM:1539:U:O2'   | 46:CM:1584:A:N3    | 2.32                     | 0.53              |
| 48:CO:90:GLU:CG    | 48:CO:97:LEU:HG    | 2.37                     | 0.53              |
| 51:CR:103:TYR:HE2  | 51:CR:184:THR:HG23 | 1.74                     | 0.53              |
| 51:CR:139:VAL:HG23 | 51:CR:150:PRO:HG3  | 1.90                     | 0.53              |
| 53:CT:218:GLU:HG2  | 53:CT:219:ARG:NH2  | 2.23                     | 0.53              |
| 61:DB:76:ILE:HD12  | 61:DB:110:ILE:HG13 | 1.90                     | 0.53              |
| 65:DF:30:TYR:O     | 65:DF:33:THR:OG1   | 2.25                     | 0.53              |
| 77:DR:24:GLN:O     | 77:DR:26:LYS:HG3   | 2.09                     | 0.53              |
| 79:DT:22:SER:CB    | 79:DT:71:ASP:HA    | 2.39                     | 0.53              |
| 79:DT:259:ILE:HG13 | 79:DT:268:LEU:HB3  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:671:U:H2'     | 1:1:672:G:C8       | 2.43                     | 0.53              |
| 1:1:1217:A:H2     | 81:P0:12:PHE:HE2   | 1.55                     | 0.53              |
| 1:1:1571:G:H2'    | 1:1:1572:G:C8      | 2.43                     | 0.53              |
| 23:5:22:PRO:HB2   | 23:5:28:PHE:HB2    | 1.91                     | 0.53              |
| 39:AL:24:ILE:HB   | 39:AL:44:LYS:HB2   | 1.90                     | 0.53              |
| 43:AP:40:LYS:HE3  | 43:AP:44:ASP:OD1   | 2.08                     | 0.53              |
| 48:D:83:LYS:NZ    | 48:D:105:PHE:O     | 2.42                     | 0.53              |
| 72:b:42:LEU:HD21  | 72:b:47:TYR:HD1    | 1.73                     | 0.53              |
| 1:AS:932:A:OP2    | 29:BV:27:LYS:HE2   | 2.08                     | 0.53              |
| 1:AS:1436:G:OP1   | 6:AY:84:HIS:NE2    | 2.39                     | 0.53              |
| 1:AS:2108:G:O4'   | 1:AS:2122:A:H4'    | 2.08                     | 0.53              |
| 1:AS:2139:G:H5''  | 4:AW:227:ARG:NH1   | 2.22                     | 0.53              |
| 1:AS:3261:A:H2'   | 1:AS:3262:U:C6     | 2.44                     | 0.53              |
| 3:AU:49:G:OP1     | 36:CC:45:HIS:HB2   | 2.08                     | 0.53              |
| 11:BD:114:ILE:HB  | 11:BD:124:ARG:HB2  | 1.91                     | 0.53              |
| 24:BQ:10:LYS:NZ   | 24:BQ:54:ALA:O     | 2.39                     | 0.53              |
| 39:CF:27:VAL:HG23 | 39:CF:41:THR:HG22  | 1.91                     | 0.53              |
| 46:CM:226:G:C6    | 46:CM:819:G:C4     | 2.96                     | 0.53              |
| 46:CM:560:G:H2'   | 46:CM:561:U:O2     | 2.09                     | 0.53              |
| 46:CM:656:C:H2'   | 46:CM:657:C:H6     | 1.74                     | 0.53              |
| 54:CU:128:PRO:HG2 | 54:CU:129:THR:HG23 | 1.90                     | 0.53              |
| 79:DT:19:TRP:HB2  | 79:DT:38:ARG:CD    | 2.39                     | 0.53              |
| 79:DT:265:ARG:HD3 | 79:DT:265:ARG:N    | 2.23                     | 0.53              |
| 1:1:487:C:H2'     | 1:1:488:G:O4'      | 2.07                     | 0.53              |
| 1:1:1684:U:H2'    | 1:1:1685:U:C6      | 2.44                     | 0.53              |
| 26:8:67:ILE:HD12  | 26:8:121:LYS:HG3   | 1.90                     | 0.53              |
| 28:AA:23:VAL:HG12 | 28:AA:45:GLY:HA3   | 1.91                     | 0.53              |
| 46:B:185:G:H3'    | 55:K:145:VAL:HG21  | 1.91                     | 0.53              |
| 46:B:1205:C:H2'   | 46:B:1206:A:C8     | 2.43                     | 0.53              |
| 46:B:1369:G:H5''  | 67:W:88:ARG:HH12   | 1.73                     | 0.53              |
| 48:D:164:VAL:HG23 | 48:D:204:ILE:HG21  | 1.91                     | 0.53              |
| 51:G:152:PRO:HG3  | 53:I:212:LEU:HD23  | 1.91                     | 0.53              |
| 52:H:113:ILE:HG23 | 52:H:191:ALA:HA    | 1.90                     | 0.53              |
| 70:Z:57:ILE:HG23  | 70:Z:58:GLY:H      | 1.73                     | 0.53              |
| 1:AS:729:C:H3'    | 1:AS:730:A:H5''    | 1.90                     | 0.53              |
| 1:AS:2131:U:OP1   | 4:AW:246:LEU:HB2   | 2.09                     | 0.53              |
| 8:BA:34:VAL:HB    | 8:BA:89:LYS:HE3    | 1.91                     | 0.53              |
| 14:BG:2:ALA:HB1   | 29:BV:33:GLY:O     | 2.08                     | 0.53              |
| 36:CC:56:THR:O    | 36:CC:60:LEU:HG    | 2.09                     | 0.53              |
| 46:CM:263:A:OP2   | 53:CT:194:LYS:NZ   | 2.41                     | 0.53              |
| 46:CM:692:U:N3    | 54:CU:92:ARG:O     | 2.34                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1160:U:H2'   | 46:CM:1161:G:H8    | 1.72                     | 0.53              |
| 46:CM:1635:A:H2'   | 46:CM:1636:C:C6    | 2.44                     | 0.53              |
| 52:CS:166:ARG:NH2  | 75:DP:45:LYS:HE3   | 2.24                     | 0.53              |
| 79:DT:238:HIS:HD2  | 79:DT:287:ILE:HG22 | 1.74                     | 0.53              |
| 79:DT:263:GLN:O    | 79:DT:264:GLU:HG2  | 2.09                     | 0.53              |
| 82:12:103:ASN:HA   | 82:12:145:GLY:N    | 2.22                     | 0.53              |
| 1:1:14:C:H5''      | 26:8:42:ARG:HG3    | 1.91                     | 0.53              |
| 1:1:1248:A:H2'     | 1:1:1249:U:H5'     | 1.90                     | 0.53              |
| 2:3:113:C:H2'      | 2:3:114:U:O4'      | 2.09                     | 0.53              |
| 45:i:132:GLU:HG2   | 50:F:91:ARG:NH2    | 2.22                     | 0.53              |
| 46:B:405:A:H2'     | 46:B:406:C:H6      | 1.73                     | 0.53              |
| 46:B:985:C:H5      | 46:B:988:A:H5''    | 1.73                     | 0.53              |
| 46:B:1012:A:OP1    | 46:B:1776:G:O2'    | 2.19                     | 0.53              |
| 46:B:1399:U:O2'    | 46:B:1400:U:OP1    | 2.27                     | 0.53              |
| 46:B:1626:C:H2'    | 46:B:1627:C:O4'    | 2.09                     | 0.53              |
| 47:C:41:ARG:HG2    | 47:C:42:PRO:HD2    | 1.91                     | 0.53              |
| 55:K:165:GLN:OE1   | 55:K:172:TYR:N     | 2.41                     | 0.53              |
| 62:R:122:THR:HG23  | 62:R:123:TYR:HD1   | 1.73                     | 0.53              |
| 64:T:99:GLN:HB2    | 64:T:118:PRO:O     | 2.09                     | 0.53              |
| 1:AS:740:A:OP1     | 19:BL:66:ARG:NH2   | 2.42                     | 0.53              |
| 1:AS:1479:G:O6     | 35:CB:4:ARG:NH2    | 2.42                     | 0.53              |
| 1:AS:1661:U:H2'    | 1:AS:1662:G:H8     | 1.73                     | 0.53              |
| 1:AS:2385:C:H2'    | 1:AS:2386:U:H6     | 1.74                     | 0.53              |
| 1:AS:2650:A:C4     | 45:CL:53:LYS:HA    | 2.43                     | 0.53              |
| 1:AS:3082:C:H2'    | 1:AS:3083:U:C6     | 2.44                     | 0.53              |
| 3:AU:5:U:H2'       | 3:AU:6:U:C6        | 2.44                     | 0.53              |
| 3:AU:10:A:H2'      | 3:AU:11:C:C6       | 2.44                     | 0.53              |
| 7:AZ:187:ALA:O     | 7:AZ:189:GLU:N     | 2.41                     | 0.53              |
| 46:CM:338:U:H2'    | 46:CM:339:A:C8     | 2.44                     | 0.53              |
| 46:CM:908:A:H2'    | 46:CM:909:A:C8     | 2.43                     | 0.53              |
| 46:CM:1072:A:H2'   | 46:CM:1073:A:C8    | 2.43                     | 0.53              |
| 46:CM:1277:G:H21   | 47:CN:111:ILE:HD11 | 1.73                     | 0.53              |
| 54:CU:4:LYS:HA     | 54:CU:38:GLN:HG2   | 1.90                     | 0.53              |
| 65:DF:22:ILE:HD11  | 65:DF:35:ILE:HG13  | 1.91                     | 0.53              |
| 82:12:143:VAL:HG12 | 82:12:151:ILE:CD1  | 2.38                     | 0.53              |
| 1:1:33:A:N3        | 1:1:806:A:O2'      | 2.42                     | 0.53              |
| 1:1:716:G:H3'      | 1:1:717:A:H5''     | 1.90                     | 0.53              |
| 1:1:1255:A:N6      | 81:P0:53:MET:HE2   | 2.24                     | 0.53              |
| 1:1:1298:A:N7      | 1:1:2829:C:O2'     | 2.41                     | 0.53              |
| 1:1:1713:U:H2'     | 1:1:1714:G:H8      | 1.72                     | 0.53              |
| 1:1:2381:G:H2'     | 1:1:2842:C:O2'     | 2.09                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:2424:U:OP1    | 37:AJ:97:ARG:NH2   | 2.41                     | 0.53              |
| 11:q:12:ILE:HD11  | 11:q:53:ILE:HG13   | 1.91                     | 0.53              |
| 31:AD:10:GLU:HB3  | 31:AD:12:ILE:HG12  | 1.90                     | 0.53              |
| 46:B:593:G:H5'    | 56:L:40:ARG:NH2    | 2.23                     | 0.53              |
| 46:B:818:U:H5'    | 46:B:819:G:H5'     | 1.90                     | 0.53              |
| 46:B:1300:U:HO2'  | 46:B:1301:G:H8     | 1.57                     | 0.53              |
| 46:B:1398:G:H4'   | 46:B:1399:U:O5'    | 2.07                     | 0.53              |
| 51:G:126:VAL:HG13 | 51:G:139:VAL:HG13  | 1.89                     | 0.53              |
| 57:M:5:LYS:NZ     | 59:O:38:HIS:CG     | 2.74                     | 0.53              |
| 79:AR:216:VAL:HA  | 79:AR:232:GLU:HA   | 1.91                     | 0.53              |
| 1:AS:164:U:H2'    | 1:AS:165:C:C6      | 2.44                     | 0.53              |
| 1:AS:663:A:H1'    | 14:BG:14:PHE:CE2   | 2.43                     | 0.53              |
| 1:AS:1525:A:P     | 1:AS:1588:G:H22    | 2.31                     | 0.53              |
| 1:AS:2322:U:H2'   | 1:AS:2323:A:C8     | 2.44                     | 0.53              |
| 1:AS:2958:U:H2'   | 1:AS:2959:A:C8     | 2.44                     | 0.53              |
| 1:AS:3261:A:H2'   | 1:AS:3262:U:H6     | 1.73                     | 0.53              |
| 5:AX:218:ILE:HB   | 5:AX:337:THR:HB    | 1.90                     | 0.53              |
| 6:AY:318:PRO:O    | 6:AY:325:LEU:HB2   | 2.09                     | 0.53              |
| 10:BC:70:LEU:HD23 | 10:BC:71:LYS:N     | 2.24                     | 0.53              |
| 25:BR:113:LYS:HZ1 | 25:BR:117:LYS:HG2  | 1.74                     | 0.53              |
| 35:CB:108:GLN:HA  | 35:CB:111:LYS:HZ3  | 1.74                     | 0.53              |
| 36:CC:77:PRO:HD2  | 36:CC:80:LEU:HD12  | 1.90                     | 0.53              |
| 46:CM:75:U:H5''   | 46:CM:76:A:OP1     | 2.09                     | 0.53              |
| 46:CM:1237:C:H4'  | 78:DS:174:MET:O    | 2.09                     | 0.53              |
| 46:CM:1302:C:O2'  | 46:CM:1386:A:N3    | 2.39                     | 0.53              |
| 46:CM:1740:A:H2'  | 46:CM:1741:A:C8    | 2.43                     | 0.53              |
| 47:CN:53:THR:OG1  | 47:CN:161:PRO:HG2  | 2.09                     | 0.53              |
| 48:CO:29:TRP:CE3  | 48:CO:45:LYS:HD3   | 2.36                     | 0.53              |
| 54:CU:168:LEU:O   | 54:CU:172:LEU:HG   | 2.09                     | 0.53              |
| 62:DC:125:PRO:HB2 | 62:DC:127:ARG:HH12 | 1.74                     | 0.53              |
| 79:DT:136:ASN:ND2 | 79:DT:138:ILE:HB   | 2.24                     | 0.53              |
| 1:1:648:C:H2'     | 1:1:649:G:C8       | 2.43                     | 0.53              |
| 1:1:1209:G:H5'    | 21:0:137:ARG:HH21  | 1.74                     | 0.53              |
| 1:1:1277:G:H5'    | 81:P0:55:LYS:HB2   | 1.91                     | 0.53              |
| 1:1:2650:A:N3     | 45:i:52:LYS:HA     | 2.23                     | 0.53              |
| 1:1:2740:U:H2'    | 1:1:2741:A:C8      | 2.44                     | 0.53              |
| 1:1:2933:G:H2'    | 1:1:2934:U:C6      | 2.44                     | 0.53              |
| 14:t:126:PHE:CD1  | 14:t:130:THR:HG21  | 2.44                     | 0.53              |
| 17:w:125:LEU:HD13 | 21:0:168:PRO:HG3   | 1.91                     | 0.53              |
| 46:B:30:G:H2'     | 46:B:31:C:C6       | 2.44                     | 0.53              |
| 46:B:444:A:N6     | 46:B:459:G:H21     | 2.07                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:945:U:H5'    | 60:P:55:ARG:HD3    | 1.89                     | 0.53              |
| 46:B:1245:U:H2'   | 46:B:1246:G:C8     | 2.44                     | 0.53              |
| 46:B:1610:C:H2'   | 46:B:1611:C:H6     | 1.72                     | 0.53              |
| 49:E:38:ARG:NH1   | 49:E:242:ALA:O     | 2.42                     | 0.53              |
| 50:F:66:ARG:HA    | 50:F:69:GLU:HG2    | 1.91                     | 0.53              |
| 62:R:94:VAL:HG21  | 62:R:116:LEU:HD11  | 1.90                     | 0.53              |
| 65:U:91:ASP:OD1   | 65:U:92:GLN:N      | 2.41                     | 0.53              |
| 1:AS:29:G:H5''    | 16:BI:188:ARG:HH12 | 1.72                     | 0.53              |
| 1:AS:683:G:P      | 14:BG:35:ARG:NH1   | 2.82                     | 0.53              |
| 1:AS:1116:A:H2'   | 1:AS:1117:U:H6     | 1.73                     | 0.53              |
| 1:AS:2959:A:H2'   | 1:AS:2960:C:H6     | 1.74                     | 0.53              |
| 3:AU:5:U:H2'      | 3:AU:6:U:H6        | 1.73                     | 0.53              |
| 10:BC:145:GLU:OE2 | 37:CD:35:ARG:NH1   | 2.41                     | 0.53              |
| 10:BC:162:GLU:CD  | 16:BI:26:ARG:HH22  | 2.17                     | 0.53              |
| 14:BG:23:ARG:NH2  | 14:BG:27:ASP:OD1   | 2.28                     | 0.53              |
| 18:BK:2:VAL:HG23  | 18:BK:3:ARG:H      | 1.74                     | 0.53              |
| 27:BT:51:ARG:HG2  | 27:BT:52:GLN:N     | 2.23                     | 0.53              |
| 46:CM:971:G:H2'   | 46:CM:972:G:O4'    | 2.07                     | 0.53              |
| 46:CM:1218:G:H22  | 46:CM:1238:U:H1'   | 1.74                     | 0.53              |
| 46:CM:1220:C:H41  | 78:DS:180:ARG:HH21 | 1.57                     | 0.53              |
| 67:DH:25:LEU:HD23 | 67:DH:88:ARG:O     | 2.08                     | 0.53              |
| 77:DR:55:LYS:HB2  | 77:DR:58:PRO:HG3   | 1.91                     | 0.53              |
| 1:1:44:A:O2'      | 1:1:94:A:N1        | 2.42                     | 0.53              |
| 1:1:659:G:P       | 29:AB:12:ARG:HH22  | 2.32                     | 0.53              |
| 1:1:1017:G:H2'    | 1:1:1018:U:O4'     | 2.08                     | 0.53              |
| 1:1:1076:A:OP2    | 7:m:140:ARG:NH2    | 2.37                     | 0.53              |
| 1:1:3171:C:H5''   | 1:1:3172:U:O5'     | 2.09                     | 0.53              |
| 3:4:21:C:OP1      | 6:l:194:LYS:NZ     | 2.32                     | 0.53              |
| 3:4:60:U:OP1      | 26:8:54:TYR:OH     | 2.25                     | 0.53              |
| 5:k:58:ARG:HH12   | 5:k:352:GLU:CD     | 2.17                     | 0.53              |
| 8:n:20:THR:HG22   | 8:n:22:LYS:H       | 1.74                     | 0.53              |
| 23:5:19:VAL:HG12  | 23:5:108:LEU:HG    | 1.90                     | 0.53              |
| 46:B:518:A:O2'    | 46:B:519:A:OP1     | 2.24                     | 0.53              |
| 46:B:1156:A:O2'   | 46:B:1557:A:N3     | 2.42                     | 0.53              |
| 46:B:1254:U:H5'   | 46:B:1418:U:OP2    | 2.08                     | 0.53              |
| 54:J:29:ASP:OD1   | 54:J:30:LEU:N      | 2.42                     | 0.53              |
| 60:P:46:THR:OG1   | 60:P:49:GLN:HG3    | 2.08                     | 0.53              |
| 79:AR:127:SER:OG  | 79:AR:129:ASP:OD1  | 2.22                     | 0.53              |
| 1:AS:428:U:H2'    | 1:AS:429:U:C6      | 2.44                     | 0.53              |
| 1:AS:498:C:H1'    | 8:BA:22:LYS:HD2    | 1.91                     | 0.53              |
| 1:AS:1592:C:H2'   | 1:AS:1593:C:C6     | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AS:2206:A:H2'   | 1:AS:2207:A:C8    | 2.44                     | 0.53              |
| 7:AZ:41:LYS:HB2   | 22:BO:68:THR:O    | 2.09                     | 0.53              |
| 13:BF:32:ARG:NH1  | 13:BF:123:TYR:OH  | 2.42                     | 0.53              |
| 14:BG:194:GLU:O   | 14:BG:198:GLU:CG  | 2.57                     | 0.53              |
| 27:BT:39:LEU:HD22 | 27:BT:43:TYR:CE2  | 2.34                     | 0.53              |
| 28:BU:34:LYS:C    | 28:BU:36:HIS:H    | 2.17                     | 0.53              |
| 46:CM:847:A:O2'   | 46:CM:948:A:N1    | 2.42                     | 0.53              |
| 46:CM:904:A:H2'   | 46:CM:905:C:C6    | 2.43                     | 0.53              |
| 46:CM:1353:G:H5'' | 66:DG:69:LYS:HE3  | 1.91                     | 0.53              |
| 59:CZ:71:ILE:O    | 59:CZ:75:VAL:HG22 | 2.08                     | 0.53              |
| 62:DC:108:LYS:HB2 | 62:DC:111:MET:HG3 | 1.90                     | 0.53              |
| 79:DT:21:THR:HB   | 79:DT:70:GLN:OE1  | 2.08                     | 0.53              |
| 1:1:693:C:H5''    | 6:1:272:LYS:HD3   | 1.92                     | 0.52              |
| 1:1:772:U:H5      | 1:1:2691:U:O2     | 1.92                     | 0.52              |
| 1:1:3314:C:H2'    | 1:1:3315:C:C6     | 2.44                     | 0.52              |
| 83:1:3401:3K5:H17 | 43:AP:57:ILE:HA   | 1.90                     | 0.52              |
| 36:AI:11:THR:HB   | 27:BT:125:LYS:HE3 | 1.91                     | 0.52              |
| 46:B:1219:A:H5''  | 46:B:1230:G:H2'   | 1.92                     | 0.52              |
| 46:B:1235:U:O2'   | 78:h:177:MET:HE2  | 2.09                     | 0.52              |
| 50:F:116:ILE:HG13 | 50:F:117:ARG:H    | 1.73                     | 0.52              |
| 60:P:46:THR:O     | 60:P:50:ILE:HD12  | 2.09                     | 0.52              |
| 1:AS:15:A:O2'     | 26:BS:45:LYS:HD2  | 2.09                     | 0.52              |
| 1:AS:294:U:OP2    | 16:BI:15:GLN:NE2  | 2.40                     | 0.52              |
| 1:AS:1852:C:H2'   | 1:AS:1853:C:H6    | 1.74                     | 0.52              |
| 1:AS:2925:U:H2'   | 1:AS:2926:U:H2'   | 1.91                     | 0.52              |
| 1:AS:3260:A:H2'   | 1:AS:3261:A:H8    | 1.71                     | 0.52              |
| 2:AT:7:G:OP1      | 7:AZ:33:ARG:NH1   | 2.42                     | 0.52              |
| 10:BC:46:ASN:HB2  | 26:BS:26:VAL:HG13 | 1.91                     | 0.52              |
| 14:BG:169:TYR:CD2 | 29:BV:132:LYS:HG3 | 2.44                     | 0.52              |
| 23:BP:37:LEU:CD1  | 23:BP:56:ILE:HD13 | 2.38                     | 0.52              |
| 23:BP:50:LEU:HG   | 23:BP:54:ILE:CD1  | 2.39                     | 0.52              |
| 27:BT:44:ASN:HB2  | 27:BT:125:LYS:HZ1 | 1.71                     | 0.52              |
| 46:CM:325:U:H2'   | 46:CM:326:A:C8    | 2.44                     | 0.52              |
| 46:CM:875:C:H2'   | 46:CM:876:A:C8    | 2.44                     | 0.52              |
| 46:CM:1396:A:O2'  | 46:CM:1397:A:OP1  | 2.23                     | 0.52              |
| 46:CM:1610:C:H2'  | 46:CM:1611:C:C6   | 2.45                     | 0.52              |
| 48:CO:220:GLN:NE2 | 48:CO:220:GLN:HA  | 2.24                     | 0.52              |
| 54:CU:29:ASP:OD1  | 54:CU:30:LEU:HD23 | 2.09                     | 0.52              |
| 54:CU:39:PHE:CD2  | 54:CU:42:ILE:HG13 | 2.44                     | 0.52              |
| 65:DF:29:MET:HB2  | 65:DF:54:LEU:HD23 | 1.89                     | 0.52              |
| 73:DN:37:LYS:O    | 73:DN:38:ARG:NH1  | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 78:DS:140:HIS:ND1 | 78:DS:143:ALA:HB2 | 2.24                     | 0.52              |
| 1:1:273:A:H2'     | 1:1:274:G:H8      | 1.73                     | 0.52              |
| 1:1:1559:C:O2'    | 1:1:1560:U:OP1    | 2.26                     | 0.52              |
| 1:1:2174:C:H2'    | 1:1:2220:A:H61    | 1.74                     | 0.52              |
| 1:1:2484:U:H2'    | 1:1:2485:U:C5     | 2.44                     | 0.52              |
| 1:1:2988:A:H2'    | 1:1:2989:A:H8     | 1.72                     | 0.52              |
| 3:4:8:C:H2'       | 3:4:9:A:H8        | 1.74                     | 0.52              |
| 30:AC:58:ARG:CG   | 30:AC:59:ALA:N    | 2.66                     | 0.52              |
| 31:AD:55:LYS:O    | 31:AD:59:GLU:HG2  | 2.09                     | 0.52              |
| 46:B:156:U:O2'    | 46:B:157:U:H3'    | 2.09                     | 0.52              |
| 46:B:257:U:OP1    | 55:K:75:LYS:NZ    | 2.34                     | 0.52              |
| 46:B:452:A:O4'    | 51:G:66:MET:HG3   | 2.08                     | 0.52              |
| 46:B:1515:U:OP1   | 52:H:109:LYS:HB2  | 2.08                     | 0.52              |
| 47:C:77:SER:HB2   | 47:C:124:THR:HG21 | 1.91                     | 0.52              |
| 50:F:52:LYS:NZ    | 50:F:90:GLU:OE1   | 2.42                     | 0.52              |
| 54:J:6:LEU:HG     | 54:J:38:GLN:HB3   | 1.91                     | 0.52              |
| 54:J:156:THR:HA   | 54:J:159:ASP:OD2  | 2.09                     | 0.52              |
| 1:AS:294:U:P      | 16:BI:15:GLN:HE22 | 2.31                     | 0.52              |
| 1:AS:409:A:H61    | 3:AU:15:G:H1'     | 1.75                     | 0.52              |
| 1:AS:1820:U:H4'   | 39:CF:17:ARG:NH1  | 2.24                     | 0.52              |
| 1:AS:2694:U:O2'   | 22:BO:88:ARG:O    | 2.17                     | 0.52              |
| 2:AT:94:C:H2'     | 2:AT:95:A:H8      | 1.73                     | 0.52              |
| 5:AX:95:THR:OG1   | 5:AX:98:GLY:O     | 2.24                     | 0.52              |
| 37:CD:3:LYS:HA    | 37:CD:11:ASN:O    | 2.09                     | 0.52              |
| 43:CJ:38:GLN:OE1  | 43:CJ:41:ARG:NH2  | 2.42                     | 0.52              |
| 46:CM:826:U:C2'   | 46:CM:827:C:H5'   | 2.38                     | 0.52              |
| 46:CM:1050:A:H5'  | 48:CO:160:LYS:NZ  | 2.24                     | 0.52              |
| 46:CM:1220:C:H5   | 78:DS:180:ARG:NE  | 2.07                     | 0.52              |
| 46:CM:1668:A:O3'  | 53:CT:31:ARG:NH2  | 2.42                     | 0.52              |
| 51:CR:141:THR:OG1 | 51:CR:143:ASP:OD1 | 2.19                     | 0.52              |
| 56:CW:53:ARG:O    | 56:CW:57:ARG:HG3  | 2.09                     | 0.52              |
| 63:DD:124:GLU:HG2 | 63:DD:133:ALA:HB1 | 1.91                     | 0.52              |
| 71:DL:10:ARG:NH1  | 71:DL:26:ASP:OD2  | 2.41                     | 0.52              |
| 79:DT:21:THR:OG1  | 79:DT:69:VAL:O    | 2.25                     | 0.52              |
| 79:DT:127:SER:OG  | 79:DT:128:ARG:N   | 2.41                     | 0.52              |
| 82:12:116:MET:HB3 | 82:12:119:LYS:HE2 | 1.91                     | 0.52              |
| 1:1:638:U:OP1     | 29:AB:21:ARG:NH1  | 2.40                     | 0.52              |
| 1:1:896:G:H1'     | 1:1:1585:A:N6     | 2.24                     | 0.52              |
| 1:1:1247:A:H2     | 82:12:139:VAL:HA  | 1.75                     | 0.52              |
| 1:1:1921:U:O2'    | 1:1:1923:G:N7     | 2.41                     | 0.52              |
| 1:1:2206:A:H2'    | 1:1:2207:A:H8     | 1.73                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:2335:A:H2'     | 1:1:2336:A:C8      | 2.44                     | 0.52              |
| 3:4:49:G:OP1       | 36:AI:45:HIS:HB2   | 2.09                     | 0.52              |
| 46:B:116:U:H2'     | 46:B:117:U:C6      | 2.45                     | 0.52              |
| 46:B:561:U:H4'     | 77:g:17:GLN:OE1    | 2.08                     | 0.52              |
| 46:B:609:U:OP2     | 70:Z:5:LYS:NZ      | 2.36                     | 0.52              |
| 49:E:220:LEU:HD23  | 69:Y:68:ARG:HA     | 1.92                     | 0.52              |
| 53:I:214:LYS:HD3   | 53:I:215:ARG:HD3   | 1.91                     | 0.52              |
| 65:U:3:LEU:HB2     | 72:b:82:GLN:OE1    | 2.10                     | 0.52              |
| 72:b:50:ILE:HG12   | 72:b:69:LEU:HD13   | 1.90                     | 0.52              |
| 1:AS:1176:A:C4     | 1:AS:1178:G:C8     | 2.98                     | 0.52              |
| 14:BG:23:ARG:NH1   | 14:BG:24:VAL:O     | 2.43                     | 0.52              |
| 14:BG:60:ALA:HB3   | 14:BG:65:TYR:O     | 2.08                     | 0.52              |
| 26:BS:126:LEU:CD1  | 26:BS:135:ILE:HD12 | 2.39                     | 0.52              |
| 36:CC:34:GLN:C     | 36:CC:38:ARG:HB2   | 2.34                     | 0.52              |
| 46:CM:78:A:H2'     | 46:CM:79:C:C6      | 2.43                     | 0.52              |
| 47:CN:133:ILE:HG12 | 47:CN:143:VAL:HG11 | 1.91                     | 0.52              |
| 62:DC:56:LEU:O     | 62:DC:60:LEU:HG    | 2.09                     | 0.52              |
| 70:DK:107:PHE:CE1  | 70:DK:120:VAL:HG12 | 2.44                     | 0.52              |
| 71:DL:55:VAL:HG22  | 71:DL:75:ILE:HG12  | 1.91                     | 0.52              |
| 73:DN:26:CYS:CB    | 73:DN:77:CYS:SG    | 2.96                     | 0.52              |
| 79:DT:5:GLU:HA     | 79:DT:313:MET:O    | 2.09                     | 0.52              |
| 79:DT:14:GLU:OE1   | 79:DT:14:GLU:N     | 2.40                     | 0.52              |
| 1:1:337:G:O4'      | 6:l:49:GLN:NE2     | 2.43                     | 0.52              |
| 1:1:559:C:H2'      | 1:1:560:C:H6       | 1.75                     | 0.52              |
| 1:1:602:A:H2'      | 1:1:603:C:H6       | 1.74                     | 0.52              |
| 1:1:671:U:O4       | 19:y:56:LYS:NZ     | 2.41                     | 0.52              |
| 1:1:1104:U:H2'     | 1:1:1105:U:H6      | 1.73                     | 0.52              |
| 1:1:3298:G:N2      | 1:1:3334:G:O2'     | 2.42                     | 0.52              |
| 16:v:164:LEU:O     | 16:v:169:LYS:NZ    | 2.40                     | 0.52              |
| 27:9:55:GLU:HB2    | 27:9:108:LYS:HB3   | 1.91                     | 0.52              |
| 46:B:78:A:H2'      | 46:B:79:C:H6       | 1.73                     | 0.52              |
| 46:B:443:A:H1'     | 46:B:523:A:H5'     | 1.90                     | 0.52              |
| 63:S:30:ILE:N      | 63:S:33:SER:O      | 2.28                     | 0.52              |
| 79:AR:218:ILE:HG23 | 79:AR:230:THR:HG22 | 1.91                     | 0.52              |
| 1:AS:547:U:H2'     | 1:AS:548:G:H8      | 1.74                     | 0.52              |
| 1:AS:2370:C:H1'    | 5:AX:266:ARG:NH2   | 2.23                     | 0.52              |
| 1:AS:2587:G:H2'    | 1:AS:2588:C:C6     | 2.44                     | 0.52              |
| 6:AY:60:GLN:O      | 38:CE:52:LYS:NZ    | 2.34                     | 0.52              |
| 6:AY:281:ILE:HB    | 19:BL:104:LEU:HD22 | 1.90                     | 0.52              |
| 14:BG:131:LYS:O    | 14:BG:135:VAL:HG23 | 2.09                     | 0.52              |
| 25:BR:88:GLU:HA    | 25:BR:91:LYS:HB3   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:CM:878:U:H5'   | 46:CM:879:U:OP2    | 2.09                     | 0.52              |
| 46:CM:903:U:H2'   | 46:CM:904:A:H8     | 1.74                     | 0.52              |
| 46:CM:1383:U:O2'  | 46:CM:1386:A:N6    | 2.32                     | 0.52              |
| 48:CO:178:ASN:OD1 | 48:CO:187:LYS:HE3  | 2.09                     | 0.52              |
| 50:CQ:28:ARG:HB3  | 57:CX:58:GLN:HE21  | 1.73                     | 0.52              |
| 67:DH:23:ILE:HG12 | 67:DH:115:VAL:HG13 | 1.91                     | 0.52              |
| 79:DT:221:ASP:OD1 | 79:DT:223:ASN:ND2  | 2.39                     | 0.52              |
| 82:12:104:ILE:HA  | 82:12:106:LEU:HD22 | 1.91                     | 0.52              |
| 1:1:299:G:C8      | 37:AJ:30:GLY:HA3   | 2.45                     | 0.52              |
| 1:1:2204:U:H2'    | 1:1:2205:C:C6      | 2.45                     | 0.52              |
| 3:4:99:C:OP1      | 26:8:53:HIS:NE2    | 2.40                     | 0.52              |
| 5:k:133:TYR:CD1   | 5:k:136:LYS:HD2    | 2.44                     | 0.52              |
| 11:q:10:LEU:HD11  | 11:q:75:ILE:HG21   | 1.91                     | 0.52              |
| 13:s:141:ARG:O    | 13:s:145:ARG:HG2   | 2.10                     | 0.52              |
| 36:AI:102:GLU:HG2 | 36:AI:106:LYS:HE3  | 1.92                     | 0.52              |
| 46:B:151:G:C6     | 46:B:160:A:C6      | 2.97                     | 0.52              |
| 48:D:111:ARG:HB3  | 73:c:68:TYR:HB2    | 1.91                     | 0.52              |
| 57:M:77:ARG:NH2   | 57:M:86:ILE:HA     | 2.24                     | 0.52              |
| 57:M:87:LEU:HD22  | 57:M:91:ARG:O      | 2.10                     | 0.52              |
| 1:AS:200:A:H2'    | 1:AS:201:G:H8      | 1.73                     | 0.52              |
| 1:AS:638:U:OP2    | 33:BZ:39:ILE:HG12  | 2.09                     | 0.52              |
| 1:AS:1794:A:H2'   | 1:AS:1795:A:C8     | 2.44                     | 0.52              |
| 1:AS:2381:G:H2'   | 1:AS:2842:C:O2'    | 2.10                     | 0.52              |
| 10:BC:42:GLN:HB3  | 10:BC:45:ARG:HH21  | 1.73                     | 0.52              |
| 10:BC:79:PHE:HA   | 10:BC:180:ILE:HG21 | 1.91                     | 0.52              |
| 80:BE:53:VAL:HG21 | 80:BE:166:ILE:HD12 | 1.91                     | 0.52              |
| 13:BF:85:LYS:HG2  | 62:DC:12:PHE:HE1   | 1.68                     | 0.52              |
| 39:CF:12:VAL:O    | 39:CF:16:ARG:HD2   | 2.09                     | 0.52              |
| 46:CM:217:A:N7    | 46:CM:816:U:O2     | 2.42                     | 0.52              |
| 46:CM:473:A:OP1   | 56:CW:126:ARG:HD3  | 2.10                     | 0.52              |
| 46:CM:932:U:H2'   | 46:CM:933:A:H8     | 1.73                     | 0.52              |
| 48:CO:97:LEU:HD21 | 48:CO:228:LEU:CD2  | 2.40                     | 0.52              |
| 48:CO:167:LYS:O   | 48:CO:171:ILE:HD12 | 2.09                     | 0.52              |
| 50:CQ:72:SER:O    | 50:CQ:76:LYS:HD2   | 2.10                     | 0.52              |
| 52:CS:54:LYS:HZ1  | 52:CS:135:ASP:CG   | 2.17                     | 0.52              |
| 57:CX:8:ARG:O     | 57:CX:12:HIS:ND1   | 2.42                     | 0.52              |
| 59:CZ:63:CYS:SG   | 59:CZ:93:ASP:O     | 2.66                     | 0.52              |
| 62:DC:50:ASP:C    | 62:DC:52:LYS:H     | 2.17                     | 0.52              |
| 67:DH:32:GLN:OE1  | 67:DH:32:GLN:N     | 2.41                     | 0.52              |
| 73:DN:51:ARG:NH2  | 75:DP:60:GLU:HG3   | 2.23                     | 0.52              |
| 79:DT:46:LYS:HG3  | 79:DT:59:LYS:HE2   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:169:G:C6      | 1:1:249:G:H1'      | 2.44                     | 0.52              |
| 1:1:200:A:H2'     | 1:1:201:G:H8       | 1.74                     | 0.52              |
| 1:1:997:G:O2'     | 1:1:1037:U:OP2     | 2.26                     | 0.52              |
| 1:1:1182:G:N3     | 21:0:112:ALA:HB1   | 2.24                     | 0.52              |
| 4:j:206:PRO:HG3   | 4:j:213:GLY:HA3    | 1.92                     | 0.52              |
| 16:v:90:ASN:O     | 43:AP:50:TYR:OH    | 2.23                     | 0.52              |
| 23:5:19:VAL:C     | 23:5:21:ALA:H      | 2.18                     | 0.52              |
| 45:i:71:LYS:HD3   | 46:B:1446:A:H4'    | 1.91                     | 0.52              |
| 46:B:29:U:H2'     | 46:B:30:G:C8       | 2.44                     | 0.52              |
| 46:B:217:A:H2'    | 46:B:218:A:O4'     | 2.08                     | 0.52              |
| 46:B:1129:U:H2'   | 46:B:1130:U:C6     | 2.44                     | 0.52              |
| 46:B:1602:C:N4    | 52:H:80:LYS:O      | 2.42                     | 0.52              |
| 47:C:14:ALA:O     | 47:C:18:LEU:HD12   | 2.10                     | 0.52              |
| 65:U:4:VAL:HG22   | 72:b:82:GLN:OE1    | 2.09                     | 0.52              |
| 1:AS:46:C:H5''    | 14:BG:16:LYS:HB3   | 1.92                     | 0.52              |
| 1:AS:426:G:H4'    | 33:BZ:52:PRO:HD3   | 1.92                     | 0.52              |
| 1:AS:437:G:O2'    | 1:AS:438:A:OP1     | 2.26                     | 0.52              |
| 1:AS:520:G:P      | 15:BH:70:ARG:HH22  | 2.33                     | 0.52              |
| 1:AS:2163:G:O2'   | 1:AS:2292:U:OP2    | 2.28                     | 0.52              |
| 1:AS:2186:A:O2'   | 1:AS:2187:U:H5'    | 2.09                     | 0.52              |
| 23:BP:19:VAL:HG13 | 23:BP:28:PHE:HD2   | 1.75                     | 0.52              |
| 46:CM:916:C:OP2   | 73:DN:70:LYS:NZ    | 2.42                     | 0.52              |
| 46:CM:965:G:H4'   | 46:CM:1763:A:H4'   | 1.91                     | 0.52              |
| 46:CM:1463:G:H2'  | 46:CM:1464:G:C8    | 2.45                     | 0.52              |
| 48:CO:126:THR:HA  | 48:CO:136:ARG:HA   | 1.91                     | 0.52              |
| 51:CR:55:ALA:HB2  | 51:CR:64:ILE:HD12  | 1.91                     | 0.52              |
| 52:CS:195:ALA:O   | 52:CS:199:ILE:HG13 | 2.08                     | 0.52              |
| 54:CU:41:SER:HB3  | 54:CU:57:PHE:HB2   | 1.91                     | 0.52              |
| 67:DH:81:TYR:HB3  | 76:DQ:52:PHE:HB3   | 1.91                     | 0.52              |
| 79:DT:57:ILE:HG13 | 79:DT:58:PRO:CD    | 2.36                     | 0.52              |
| 79:DT:88:ARG:NH2  | 79:DT:109:GLY:HA2  | 2.24                     | 0.52              |
| 79:DT:208:CYS:HB2 | 79:DT:222:LEU:HD11 | 1.91                     | 0.52              |
| 79:DT:235:ALA:HB3 | 79:DT:253:THR:HB   | 1.90                     | 0.52              |
| 1:1:547:U:H2'     | 1:1:548:G:H8       | 1.74                     | 0.52              |
| 1:1:656:G:N2      | 6:l:94:MET:HB2     | 2.25                     | 0.52              |
| 1:1:1593:C:H2'    | 1:1:1594:G:C8      | 2.45                     | 0.52              |
| 1:1:1852:C:H2'    | 1:1:1853:C:H6      | 1.73                     | 0.52              |
| 1:1:2107:U:H2'    | 1:1:2108:G:C8      | 2.45                     | 0.52              |
| 1:1:2404:U:H2'    | 1:1:2405:U:C6      | 2.45                     | 0.52              |
| 1:1:2796:G:H2'    | 1:1:2797:C:C6      | 2.45                     | 0.52              |
| 1:1:3082:C:H2'    | 1:1:3083:U:C6      | 2.44                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:4:63:G:O2'      | 36:AI:49:LYS:NZ    | 2.35                     | 0.52              |
| 46:B:530:U:OP1    | 71:a:64:PHE:HA     | 2.10                     | 0.52              |
| 46:B:1102:U:H2'   | 46:B:1103:G:H8     | 1.75                     | 0.52              |
| 1:AS:1617:A:H2'   | 1:AS:1618:U:H6     | 1.73                     | 0.52              |
| 1:AS:2197:A:H2'   | 1:AS:2198:A:C8     | 2.45                     | 0.52              |
| 1:AS:3005:A:H2    | 11:BD:120:GLU:HG2  | 1.74                     | 0.52              |
| 1:AS:3067:U:H2'   | 1:AS:3068:C:H6     | 1.75                     | 0.52              |
| 1:AS:3240:U:OP2   | 34:CA:66:VAL:HG21  | 2.09                     | 0.52              |
| 45:CL:48:PRO:HA   | 45:CL:51:ALA:HB3   | 1.92                     | 0.52              |
| 46:CM:415:A:H5'   | 46:CM:416:G:C4     | 2.43                     | 0.52              |
| 46:CM:931:U:H2'   | 46:CM:932:U:C6     | 2.45                     | 0.52              |
| 47:CN:47:ILE:HD12 | 64:DE:106:THR:HG22 | 1.90                     | 0.52              |
| 48:CO:127:VAL:N   | 48:CO:135:LEU:O    | 2.30                     | 0.52              |
| 51:CR:100:ARG:NH1 | 51:CR:118:GLU:OE2  | 2.43                     | 0.52              |
| 54:CU:72:ARG:HA   | 54:CU:75:ARG:HE    | 1.74                     | 0.52              |
| 76:DQ:17:GLY:HA2  | 76:DQ:27:HIS:ND1   | 2.24                     | 0.52              |
| 79:DT:117:ALA:HA  | 79:DT:157:ILE:CD1  | 2.38                     | 0.52              |
| 79:DT:302:TYR:CE2 | 79:DT:308:ARG:HB2  | 2.44                     | 0.52              |
| 82:12:108:GLU:HG3 | 82:12:111:GLU:OE1  | 2.08                     | 0.52              |
| 1:1:2090:U:H4'    | 1:1:2091:A:O5'     | 2.08                     | 0.52              |
| 1:1:2405:U:H2'    | 1:1:2406:U:C6      | 2.44                     | 0.52              |
| 1:1:2428:G:N2     | 1:1:2475:U:H3      | 2.08                     | 0.52              |
| 1:1:2718:A:H5'    | 7:m:178:ASN:OD1    | 2.10                     | 0.52              |
| 20:z:172:ARG:HH21 | 46:B:837:C:P       | 2.32                     | 0.52              |
| 25:7:90:ILE:O     | 25:7:94:ARG:HG3    | 2.09                     | 0.52              |
| 46:B:654:G:H3'    | 46:B:655:U:C6      | 2.45                     | 0.52              |
| 46:B:1455:A:H2'   | 46:B:1456:C:C6     | 2.45                     | 0.52              |
| 46:B:1529:G:H5''  | 66:V:87:GLY:C      | 2.34                     | 0.52              |
| 48:D:56:ASN:OD1   | 48:D:57:ALA:N      | 2.42                     | 0.52              |
| 51:G:71:GLN:HB2   | 51:G:91:THR:HB     | 1.91                     | 0.52              |
| 79:AR:214:ASP:OD1 | 79:AR:214:ASP:N    | 2.42                     | 0.52              |
| 1:AS:258:U:H2'    | 1:AS:259:C:C6      | 2.44                     | 0.52              |
| 1:AS:1391:G:O2'   | 3:AU:18:U:O2       | 2.28                     | 0.52              |
| 1:AS:2485:U:H2'   | 1:AS:2486:U:C6     | 2.44                     | 0.52              |
| 10:BC:115:ALA:O   | 10:BC:118:ALA:HB3  | 2.10                     | 0.52              |
| 46:CM:498:C:H1'   | 46:CM:499:U:H5''   | 1.91                     | 0.52              |
| 46:CM:946:U:H5''  | 60:DA:71:ILE:HD12  | 1.92                     | 0.52              |
| 46:CM:975:C:H1'   | 61:DB:122:ARG:HG2  | 1.91                     | 0.52              |
| 46:CM:1399:U:O2'  | 46:CM:1400:U:OP1   | 2.28                     | 0.52              |
| 65:DF:83:ALA:HB1  | 65:DF:97:ASP:OD2   | 2.10                     | 0.52              |
| 79:DT:164:SER:HB2 | 79:DT:180:LEU:HB2  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:739:C:H5''    | 19:y:69:ARG:HH22   | 1.75                     | 0.52              |
| 46:B:154:A:H2'    | 46:B:155:A:O4'     | 2.10                     | 0.52              |
| 46:B:245:A:O2'    | 58:N:37:ASP:O      | 2.25                     | 0.52              |
| 46:B:384:G:H2'    | 46:B:385:A:C8      | 2.45                     | 0.52              |
| 46:B:931:U:H2'    | 46:B:932:U:C6      | 2.45                     | 0.52              |
| 46:B:1335:U:H2'   | 46:B:1336:G:H8     | 1.75                     | 0.52              |
| 50:F:141:GLY:HA3  | 50:F:183:LEU:HD23  | 1.92                     | 0.52              |
| 54:J:25:GLU:CD    | 54:J:35:ARG:HH22   | 2.17                     | 0.52              |
| 54:J:30:LEU:HD12  | 54:J:34:LEU:HD11   | 1.92                     | 0.52              |
| 54:J:92:ARG:HH12  | 54:J:120:LYS:HB3   | 1.74                     | 0.52              |
| 60:P:20:ARG:NH2   | 69:Y:56:HIS:HB3    | 2.25                     | 0.52              |
| 64:T:89:SER:HB3   | 64:T:92:ASP:HB2    | 1.92                     | 0.52              |
| 79:AR:42:LEU:HB2  | 79:AR:62:PHE:HB2   | 1.91                     | 0.52              |
| 1:AS:1801:C:O2'   | 35:CB:76:TYR:HA    | 2.09                     | 0.52              |
| 1:AS:2244:U:H2'   | 1:AS:2245:C:H6     | 1.75                     | 0.52              |
| 1:AS:2853:C:H2'   | 1:AS:2854:U:H6     | 1.72                     | 0.52              |
| 1:AS:3302:G:H2'   | 1:AS:3303:C:C6     | 2.45                     | 0.52              |
| 2:AT:70:A:H2'     | 2:AT:71:U:H6       | 1.73                     | 0.52              |
| 39:CF:38:PHE:HE1  | 39:CF:57:ASN:HB3   | 1.74                     | 0.52              |
| 39:CF:58:ASP:HB3  | 39:CF:61:LYS:HB3   | 1.91                     | 0.52              |
| 46:CM:829:A:H2'   | 46:CM:830:G:H8     | 1.74                     | 0.52              |
| 46:CM:1600:U:OP2  | 52:CS:84:LYS:NZ    | 2.37                     | 0.52              |
| 46:CM:1750:A:H5'' | 46:CM:1758:U:H5''  | 1.92                     | 0.52              |
| 50:CQ:9:LYS:HD3   | 67:DH:60:LYS:HD3   | 1.90                     | 0.52              |
| 51:CR:150:PRO:O   | 53:CT:208:TYR:HE1  | 1.93                     | 0.52              |
| 58:CY:77:SER:HB3  | 58:CY:85:ILE:HB    | 1.92                     | 0.52              |
| 59:CZ:42:ALA:HB3  | 59:CZ:122:VAL:HB   | 1.92                     | 0.52              |
| 59:CZ:69:GLU:O    | 59:CZ:72:ILE:N     | 2.31                     | 0.52              |
| 63:DD:86:LYS:HG2  | 63:DD:116:LEU:HD13 | 1.91                     | 0.52              |
| 79:DT:143:ALA:HB2 | 79:DT:183:TYR:CZ   | 2.45                     | 0.52              |
| 79:DT:192:HIS:CD2 | 79:DT:218:ILE:HD12 | 2.45                     | 0.52              |
| 1:1:249:G:N2      | 1:1:251:G:N7       | 2.58                     | 0.52              |
| 1:1:403:C:O2'     | 1:1:404:G:OP1      | 2.26                     | 0.52              |
| 1:1:407:A:C2      | 3:4:17:A:H1'       | 2.45                     | 0.52              |
| 1:1:437:G:O2'     | 1:1:438:A:OP1      | 2.28                     | 0.52              |
| 1:1:1377:A:H2'    | 1:1:1378:G:C8      | 2.45                     | 0.52              |
| 1:1:1377:A:H2'    | 1:1:1378:G:H8      | 1.74                     | 0.52              |
| 1:1:1466:U:O3'    | 20:z:5:ARG:NH2     | 2.42                     | 0.52              |
| 1:1:1489:G:OP2    | 1:1:1489:G:N2      | 2.38                     | 0.52              |
| 3:4:37:A:OP2      | 36:AI:86:ARG:HD2   | 2.10                     | 0.52              |
| 46:B:283:G:H2'    | 46:B:284:C:C6      | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:1241:A:H5'   | 46:B:1242:U:C5    | 2.45                     | 0.52              |
| 46:B:1265:C:O2'   | 67:W:69:THR:HG22  | 2.09                     | 0.52              |
| 46:B:1577:G:OP1   | 66:V:91:HIS:HB2   | 2.10                     | 0.52              |
| 78:h:149:LYS:O    | 78:h:157:GLU:HB2  | 2.10                     | 0.52              |
| 1:AS:11:A:H4'     | 26:BS:34:LEU:HD21 | 1.92                     | 0.52              |
| 1:AS:1899:U:O2'   | 1:AS:1901:G:N7    | 2.40                     | 0.52              |
| 1:AS:2625:C:OP1   | 43:CJ:89:LYS:HB2  | 2.10                     | 0.52              |
| 1:AS:2937:U:O2'   | 4:AW:221:LYS:HD3  | 2.09                     | 0.52              |
| 21:BN:12:ARG:HB3  | 21:BN:24:LEU:HD23 | 1.91                     | 0.52              |
| 26:BS:134:ASP:O   | 26:BS:138:ARG:HG3 | 2.10                     | 0.52              |
| 46:CM:1486:G:OP2  | 66:DG:73:VAL:HG12 | 2.09                     | 0.52              |
| 47:CN:15:LYS:HZ3  | 64:DE:93:LEU:HD22 | 1.74                     | 0.52              |
| 50:CQ:28:ARG:HB3  | 57:CX:58:GLN:NE2  | 2.24                     | 0.52              |
| 52:CS:41:LYS:HB3  | 52:CS:46:TRP:O    | 2.10                     | 0.52              |
| 59:CZ:75:VAL:O    | 59:CZ:78:LEU:HB2  | 2.10                     | 0.52              |
| 79:DT:221:ASP:O   | 79:DT:225:ASN:N   | 2.41                     | 0.52              |
| 1:1:2184:G:O2'    | 1:1:2187:U:O4     | 2.23                     | 0.51              |
| 1:1:3093:U:H1'    | 1:1:3094:A:H5''   | 1.92                     | 0.51              |
| 14:t:158:LEU:HB3  | 29:AB:98:ALA:HB1  | 1.92                     | 0.51              |
| 38:AK:25:ARG:HH11 | 40:AM:50:GLY:HA2  | 1.75                     | 0.51              |
| 46:B:216:A:O2'    | 46:B:217:A:O5'    | 2.28                     | 0.51              |
| 46:B:1141:C:H2'   | 46:B:1142:A:C8    | 2.44                     | 0.51              |
| 48:D:180:THR:N    | 48:D:183:GLN:OE1  | 2.43                     | 0.51              |
| 1:AS:710:G:OP1    | 14:BG:176:ARG:NH1 | 2.43                     | 0.51              |
| 1:AS:1746:A:H1'   | 1:AS:1748:A:N7    | 2.26                     | 0.51              |
| 1:AS:2855:U:H2'   | 1:AS:2856:C:H6    | 1.75                     | 0.51              |
| 1:AS:2988:A:H2'   | 1:AS:2989:A:C8    | 2.44                     | 0.51              |
| 1:AS:3207:G:N2    | 1:AS:3210:A:OP2   | 2.43                     | 0.51              |
| 1:AS:3245:A:O2'   | 1:AS:3246:C:H6    | 1.92                     | 0.51              |
| 2:AT:4:U:H2'      | 2:AT:5:G:C8       | 2.44                     | 0.51              |
| 10:BC:219:ILE:O   | 10:BC:223:TYR:HD2 | 1.93                     | 0.51              |
| 28:BU:87:LEU:HD12 | 28:BU:88:ASP:N    | 2.23                     | 0.51              |
| 37:CD:59:LEU:HD13 | 37:CD:67:ARG:NH1  | 2.26                     | 0.51              |
| 46:CM:1498:G:H2'  | 46:CM:1499:G:H8   | 1.75                     | 0.51              |
| 46:CM:1602:C:H5'' | 46:CM:1603:G:O5'  | 2.10                     | 0.51              |
| 52:CS:36:ALA:HB2  | 52:CS:44:ASN:OD1  | 2.10                     | 0.51              |
| 52:CS:139:ASN:O   | 52:CS:214:LYS:NZ  | 2.42                     | 0.51              |
| 54:CU:156:THR:HA  | 54:CU:159:ASP:OD1 | 2.10                     | 0.51              |
| 55:CV:38:ILE:HG12 | 55:CV:96:LEU:HD11 | 1.92                     | 0.51              |
| 64:DE:90:ALA:HA   | 64:DE:95:HIS:CD2  | 2.44                     | 0.51              |
| 70:DK:126:LYS:HG2 | 70:DK:131:SER:HA  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:DT:50:GLY:N     | 79:DT:55:TYR:HA    | 2.23                     | 0.51              |
| 82:12:109:ILE:HD13 | 82:12:112:ILE:HD12 | 1.92                     | 0.51              |
| 6:l:114:VAL:HB     | 6:l:119:LYS:HE3    | 1.91                     | 0.51              |
| 36:AI:86:ARG:O     | 36:AI:90:ARG:HD3   | 2.10                     | 0.51              |
| 46:B:252:A:H2'     | 46:B:253:U:H6      | 1.75                     | 0.51              |
| 46:B:671:G:H3'     | 46:B:672:U:C5'     | 2.35                     | 0.51              |
| 46:B:1341:U:H1'    | 46:B:1353:G:N2     | 2.25                     | 0.51              |
| 46:B:1596:U:OP1    | 63:S:75:SER:N      | 2.35                     | 0.51              |
| 53:I:180:THR:HG23  | 53:I:183:THR:H     | 1.75                     | 0.51              |
| 62:R:26:VAL:HG23   | 62:R:27:GLU:HG3    | 1.91                     | 0.51              |
| 63:S:124:GLU:HG2   | 63:S:133:ALA:HB1   | 1.91                     | 0.51              |
| 71:a:6:THR:HB      | 71:a:28:LEU:HB2    | 1.91                     | 0.51              |
| 1:AS:634:C:O2      | 1:AS:2355:G:O2'    | 2.22                     | 0.51              |
| 13:BF:117:ASP:HB3  | 13:BF:120:ILE:HD12 | 1.91                     | 0.51              |
| 18:BK:40:LYS:HD2   | 18:BK:113:VAL:HG22 | 1.92                     | 0.51              |
| 27:BT:80:ILE:HG23  | 27:BT:101:PRO:HG3  | 1.91                     | 0.51              |
| 36:CC:70:TYR:HA    | 36:CC:73:LYS:HG3   | 1.92                     | 0.51              |
| 37:CD:87:GLU:O     | 37:CD:88:GLU:C     | 2.53                     | 0.51              |
| 45:CL:46:ALA:O     | 45:CL:47:ASP:C     | 2.52                     | 0.51              |
| 45:CL:156:ALA:O    | 57:CX:17:GLN:NE2   | 2.44                     | 0.51              |
| 48:CO:42:ASN:O     | 48:CO:43:VAL:C     | 2.54                     | 0.51              |
| 50:CQ:116:ILE:HD12 | 50:CQ:153:TYR:OH   | 2.10                     | 0.51              |
| 59:CZ:51:ALA:HB3   | 59:CZ:122:VAL:HG11 | 1.92                     | 0.51              |
| 65:DF:36:ARG:NH1   | 65:DF:105:LEU:HD22 | 2.25                     | 0.51              |
| 79:DT:285:GLU:O    | 79:DT:303:THR:HG23 | 2.10                     | 0.51              |
| 81:P0:64:ARG:HA    | 81:P0:77:LEU:CD1   | 2.40                     | 0.51              |
| 1:1:293:C:O2'      | 37:AJ:75:ARG:HA    | 2.11                     | 0.51              |
| 1:1:506:A:OP2      | 34:AG:39:LYS:HG3   | 2.11                     | 0.51              |
| 1:1:2370:C:H1'     | 5:k:266:ARG:NH2    | 2.25                     | 0.51              |
| 5:k:57:VAL:HG12    | 5:k:357:LYS:HB2    | 1.93                     | 0.51              |
| 5:k:313:ARG:O      | 5:k:333:LYS:HE3    | 2.10                     | 0.51              |
| 39:AL:34:ASN:ND2   | 39:AL:34:ASN:O     | 2.42                     | 0.51              |
| 46:B:1024:A:O2'    | 46:B:1025:G:O5'    | 2.26                     | 0.51              |
| 46:B:1553:U:H5''   | 65:U:39:GLY:H      | 1.75                     | 0.51              |
| 46:B:1582:U:H5'    | 46:B:1583:C:OP2    | 2.10                     | 0.51              |
| 50:F:71:THR:HB     | 50:F:87:ILE:HD12   | 1.92                     | 0.51              |
| 51:G:11:ARG:HA     | 51:G:28:ALA:HB2    | 1.93                     | 0.51              |
| 51:G:100:ARG:HG2   | 51:G:102:VAL:HG13  | 1.91                     | 0.51              |
| 75:e:19:THR:HG23   | 75:e:25:VAL:HG13   | 1.92                     | 0.51              |
| 1:AS:40:G:N2       | 1:AS:2775:A:H62    | 2.08                     | 0.51              |
| 1:AS:146:U:OP1     | 10:BC:197:ALA:N    | 2.38                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AS:1593:C:H2'   | 1:AS:1594:G:C8     | 2.46                     | 0.51              |
| 1:AS:2854:U:H2'   | 1:AS:2855:U:C6     | 2.45                     | 0.51              |
| 3:AU:63:G:N2      | 3:AU:97:A:N1       | 2.54                     | 0.51              |
| 5:AX:219:ALA:HB3  | 5:AX:329:PRO:HG2   | 1.92                     | 0.51              |
| 7:AZ:41:LYS:NZ    | 22:BO:32:LYS:O     | 2.43                     | 0.51              |
| 17:BJ:63:THR:HG23 | 17:BJ:66:ASN:O     | 2.10                     | 0.51              |
| 28:BU:116:LYS:O   | 28:BU:116:LYS:NZ   | 2.40                     | 0.51              |
| 37:CD:87:GLU:O    | 37:CD:90:THR:N     | 2.43                     | 0.51              |
| 46:CM:1024:A:O2'  | 46:CM:1025:G:O5'   | 2.25                     | 0.51              |
| 49:CP:97:VAL:HG11 | 49:CP:124:ILE:HG12 | 1.91                     | 0.51              |
| 54:CU:10:PRO:HG2  | 54:CU:15:LEU:HD11  | 1.92                     | 0.51              |
| 63:DD:93:GLN:O    | 79:DT:60:LYS:HE2   | 2.10                     | 0.51              |
| 79:DT:65:HIS:H    | 79:DT:93:TRP:HH2   | 1.58                     | 0.51              |
| 1:1:212:A:O4'     | 27:9:2:ALA:HA      | 2.10                     | 0.51              |
| 1:1:1011:C:O5'    | 1:1:1011:C:H6      | 1.93                     | 0.51              |
| 1:1:1021:A:H2'    | 1:1:1022:A:C8      | 2.45                     | 0.51              |
| 1:1:1029:U:H2'    | 1:1:1030:U:C6      | 2.45                     | 0.51              |
| 1:1:1809:A:OP1    | 1:1:1813:G:O2'     | 2.25                     | 0.51              |
| 1:1:1852:C:C2     | 1:1:1853:C:C5      | 2.98                     | 0.51              |
| 1:1:2086:C:H1'    | 1:1:3309:A:H8      | 1.73                     | 0.51              |
| 1:1:3320:U:H5''   | 1:1:3321:G:OP1     | 2.10                     | 0.51              |
| 17:w:13:LYS:HD2   | 17:w:38:ARG:NH2    | 2.25                     | 0.51              |
| 19:y:67:ILE:HG12  | 19:y:81:ILE:HG21   | 1.92                     | 0.51              |
| 45:i:134:GLU:O    | 45:i:135:GLU:C     | 2.52                     | 0.51              |
| 46:B:150:U:O2     | 53:I:4:ASN:ND2     | 2.38                     | 0.51              |
| 46:B:167:A:H8     | 46:B:167:A:OP2     | 1.93                     | 0.51              |
| 46:B:885:A:H2'    | 46:B:886:G:H8      | 1.76                     | 0.51              |
| 46:B:1084:U:OP1   | 69:Y:71:LYS:NZ     | 2.36                     | 0.51              |
| 74:d:31:PHE:CD1   | 74:d:81:ARG:HG3    | 2.46                     | 0.51              |
| 1:AS:164:U:H2'    | 1:AS:165:C:H6      | 1.75                     | 0.51              |
| 1:AS:520:G:OP1    | 15:BH:70:ARG:NH2   | 2.35                     | 0.51              |
| 1:AS:561:U:OP1    | 21:BN:68:LYS:HG3   | 2.11                     | 0.51              |
| 1:AS:583:A:H2'    | 1:AS:584:C:H6      | 1.76                     | 0.51              |
| 1:AS:1338:G:H2'   | 1:AS:1339:A:O4'    | 2.11                     | 0.51              |
| 1:AS:2347:G:H2'   | 1:AS:2348:G:C8     | 2.45                     | 0.51              |
| 11:BD:31:ARG:HB2  | 11:BD:82:VAL:HA    | 1.91                     | 0.51              |
| 80:BE:101:LYS:HE2 | 80:BE:101:LYS:HA   | 1.91                     | 0.51              |
| 25:BR:102:LYS:CE  | 25:BR:105:ARG:HH22 | 2.20                     | 0.51              |
| 28:BU:96:VAL:O    | 28:BU:96:VAL:HG12  | 2.11                     | 0.51              |
| 39:CF:49:ARG:NH1  | 39:CF:50:TYR:CE2   | 2.79                     | 0.51              |
| 46:CM:188:U:H2'   | 46:CM:189:G:C8     | 2.45                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:CM:216:A:H61   | 46:CM:829:A:H4'    | 1.75                     | 0.51              |
| 46:CM:1183:G:O4'  | 67:DH:72:GLY:HA3   | 2.09                     | 0.51              |
| 46:CM:1529:G:H5'' | 66:DG:87:GLY:C     | 2.35                     | 0.51              |
| 46:CM:1584:A:C8   | 76:DQ:14:PHE:HD1   | 2.28                     | 0.51              |
| 46:CM:1780:G:N2   | 73:DN:76:SER:OG    | 2.43                     | 0.51              |
| 63:DD:38:VAL:O    | 63:DD:44:ARG:NH2   | 2.41                     | 0.51              |
| 70:DK:48:HIS:HB3  | 70:DK:103:LEU:HD11 | 1.91                     | 0.51              |
| 79:DT:265:ARG:HD3 | 79:DT:265:ARG:H    | 1.73                     | 0.51              |
| 82:12:122:GLY:HA3 | 82:12:127:SER:HB2  | 1.92                     | 0.51              |
| 1:1:158:A:H2'     | 1:1:159:A:H8       | 1.75                     | 0.51              |
| 1:1:245:G:H3'     | 1:1:246:U:H6       | 1.75                     | 0.51              |
| 1:1:3150:A:C4     | 17:w:115:LYS:HA    | 2.46                     | 0.51              |
| 9:o:130:PRO:HG2   | 9:o:131:TYR:CE2    | 2.45                     | 0.51              |
| 11:q:25:VAL:O     | 11:q:35:THR:HA     | 2.09                     | 0.51              |
| 46:B:643:U:H2'    | 46:B:644:U:O4'     | 2.11                     | 0.51              |
| 46:B:961:G:N1     | 46:B:1008:A:O2'    | 2.40                     | 0.51              |
| 46:B:1167:U:O2'   | 46:B:1169:A:N7     | 2.41                     | 0.51              |
| 46:B:1672:G:H2'   | 46:B:1673:U:C6     | 2.45                     | 0.51              |
| 46:B:1743:A:C8    | 46:B:1743:A:H5''   | 2.45                     | 0.51              |
| 62:R:14:GLN:HE22  | 62:R:23:LYS:HB2    | 1.75                     | 0.51              |
| 67:W:32:GLN:HB3   | 67:W:108:GLU:HG2   | 1.92                     | 0.51              |
| 79:AR:235:ALA:HB3 | 79:AR:253:THR:HB   | 1.92                     | 0.51              |
| 1:AS:243:G:H2'    | 1:AS:244:G:H8      | 1.74                     | 0.51              |
| 1:AS:1130:G:O2'   | 1:AS:2614:A:N3     | 2.37                     | 0.51              |
| 1:AS:2650:A:C5    | 45:CL:53:LYS:HA    | 2.46                     | 0.51              |
| 3:AU:126:A:O2'    | 3:AU:129:C:N4      | 2.44                     | 0.51              |
| 25:BR:120:LYS:HA  | 25:BR:123:ARG:HB2  | 1.91                     | 0.51              |
| 37:CD:69:LYS:HD2  | 37:CD:83:LEU:HD23  | 1.93                     | 0.51              |
| 46:CM:12:U:H2'    | 46:CM:13:C:H6      | 1.76                     | 0.51              |
| 46:CM:1062:C:H2'  | 46:CM:1063:C:H6    | 1.76                     | 0.51              |
| 46:CM:1317:C:O2'  | 50:CQ:163:GLN:HB3  | 2.11                     | 0.51              |
| 46:CM:1454:U:O2'  | 66:DG:87:GLY:O     | 2.25                     | 0.51              |
| 52:CS:168:VAL:O   | 52:CS:172:ILE:HG13 | 2.11                     | 0.51              |
| 54:CU:16:LYS:N    | 54:CU:16:LYS:HD2   | 2.25                     | 0.51              |
| 79:DT:143:ALA:HB2 | 79:DT:183:TYR:CE2  | 2.46                     | 0.51              |
| 79:DT:291:TRP:CD2 | 79:DT:298:LEU:HD13 | 2.45                     | 0.51              |
| 81:P0:56:ASN:HB3  | 81:P0:60:ARG:NH2   | 2.25                     | 0.51              |
| 81:P0:92:ASP:O    | 81:P0:96:ILE:HG12  | 2.11                     | 0.51              |
| 1:1:158:A:H2'     | 1:1:159:A:C8       | 2.46                     | 0.51              |
| 3:4:29:U:H5''     | 14:t:27:ASP:HB3    | 1.92                     | 0.51              |
| 46:B:634:A:H5''   | 69:Y:31:SER:HB3    | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:903:U:H2'    | 46:B:904:A:H8     | 1.72                     | 0.51              |
| 46:B:1056:U:O3'   | 74:d:19:HIS:HB2   | 2.10                     | 0.51              |
| 46:B:1335:U:H5'   | 63:S:67:LYS:NZ    | 2.26                     | 0.51              |
| 47:C:118:PRO:HG2  | 47:C:141:ILE:HD13 | 1.92                     | 0.51              |
| 63:S:68:VAL:HG11  | 63:S:80:ILE:HD11  | 1.92                     | 0.51              |
| 1:AS:422:A:C2     | 1:AS:2341:A:H4'   | 2.46                     | 0.51              |
| 1:AS:1014:G:O6    | 1:AS:1030:U:O4    | 2.29                     | 0.51              |
| 1:AS:2628:A:C8    | 1:AS:2630:G:C8    | 2.99                     | 0.51              |
| 1:AS:2659:G:H4'   | 7:AZ:7:PHE:HE2    | 1.76                     | 0.51              |
| 1:AS:2667:A:O2'   | 1:AS:2668:A:OP2   | 2.28                     | 0.51              |
| 25:BR:99:SER:O    | 25:BR:102:LYS:HB2 | 2.10                     | 0.51              |
| 46:CM:933:A:H2'   | 46:CM:934:C:C6    | 2.45                     | 0.51              |
| 46:CM:1145:A:H2'  | 46:CM:1146:C:C6   | 2.44                     | 0.51              |
| 46:CM:1181:A:OP2  | 46:CM:1450:G:N2   | 2.32                     | 0.51              |
| 46:CM:1369:G:O2'  | 46:CM:1370:A:H8   | 1.92                     | 0.51              |
| 46:CM:1739:U:H2'  | 46:CM:1740:A:H8   | 1.74                     | 0.51              |
| 52:CS:122:HIS:ND1 | 52:CS:127:GLN:O   | 2.35                     | 0.51              |
| 53:CT:48:TYR:CD2  | 53:CT:117:GLY:HA3 | 2.45                     | 0.51              |
| 59:CZ:90:LYS:HG2  | 59:CZ:91:VAL:H    | 1.75                     | 0.51              |
| 1:1:897:G:OP1     | 38:AK:12:HIS:NE2  | 2.42                     | 0.51              |
| 1:1:1199:A:H2'    | 1:1:1200:A:C8     | 2.46                     | 0.51              |
| 1:1:1434:U:H4'    | 6:l:89:ALA:CB     | 2.41                     | 0.51              |
| 1:1:2451:C:OP1    | 1:1:2452:G:N2     | 2.43                     | 0.51              |
| 1:1:3152:G:H4'    | 17:w:162:LYS:HG2  | 1.93                     | 0.51              |
| 3:4:85:G:P        | 27:9:113:LYS:HZ1  | 2.32                     | 0.51              |
| 5:k:217:VAL:HG11  | 5:k:328:ILE:HB    | 1.93                     | 0.51              |
| 7:m:290:ILE:HG13  | 12:r:206:LEU:HD21 | 1.92                     | 0.51              |
| 35:AH:41:ARG:HA   | 35:AH:56:THR:HG23 | 1.92                     | 0.51              |
| 46:B:4:C:H5       | 46:B:20:G:H1      | 1.59                     | 0.51              |
| 46:B:1326:A:H1'   | 79:AR:66:SER:HB2  | 1.92                     | 0.51              |
| 52:H:63:GLN:NE2   | 52:H:66:ASN:H     | 2.08                     | 0.51              |
| 63:S:38:VAL:CG1   | 63:S:44:ARG:HG3   | 2.39                     | 0.51              |
| 66:V:30:VAL:HG13  | 66:V:34:VAL:HG11  | 1.92                     | 0.51              |
| 1:AS:249:G:H2'    | 1:AS:251:G:OP2    | 2.10                     | 0.51              |
| 1:AS:1029:U:O2'   | 1:AS:1030:U:OP1   | 2.27                     | 0.51              |
| 1:AS:1632:C:H5''  | 28:BU:73:LYS:NZ   | 2.26                     | 0.51              |
| 1:AS:2335:A:H2'   | 1:AS:2336:A:C8    | 2.45                     | 0.51              |
| 1:AS:2959:A:H2'   | 1:AS:2960:C:C6    | 2.45                     | 0.51              |
| 1:AS:3244:A:O2'   | 1:AS:3245:A:H5'   | 2.11                     | 0.51              |
| 10:BC:122:THR:HB  | 10:BC:125:ASP:OD2 | 2.10                     | 0.51              |
| 37:CD:4:SER:OG    | 37:CD:12:LYS:HA   | 2.11                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:CL:107:TRP:CE2  | 50:CQ:143:LEU:HB2  | 2.46                     | 0.51              |
| 46:CM:1265:C:H2'   | 46:CM:1266:G:C8    | 2.46                     | 0.51              |
| 46:CM:1543:A:OP1   | 62:DC:44:ARG:HD3   | 2.11                     | 0.51              |
| 49:CP:93:MET:HG3   | 49:CP:116:VAL:HG23 | 1.93                     | 0.51              |
| 51:CR:100:ARG:NH2  | 51:CR:121:TYR:O    | 2.44                     | 0.51              |
| 59:CZ:79:CYS:HA    | 59:CZ:86:ILE:HB    | 1.92                     | 0.51              |
| 62:DC:36:LEU:O     | 62:DC:36:LEU:HG    | 2.10                     | 0.51              |
| 62:DC:125:PRO:CB   | 62:DC:127:ARG:HH12 | 2.24                     | 0.51              |
| 64:DE:78:ARG:HH11  | 64:DE:81:LYS:CD    | 2.23                     | 0.51              |
| 78:DS:147:TYR:HD2  | 78:DS:160:ARG:HG2  | 1.76                     | 0.51              |
| 78:DS:163:CYS:HB3  | 78:DS:169:GLY:HA2  | 1.92                     | 0.51              |
| 79:DT:148:HIS:NE2  | 79:DT:176:LYS:HB2  | 2.26                     | 0.51              |
| 79:DT:158:SER:HB2  | 79:DT:160:SER:OG   | 2.11                     | 0.51              |
| 82:12:125:LEU:HD11 | 82:12:164:GLU:HB2  | 1.92                     | 0.51              |
| 1:1:1568:U:C4      | 1:1:1569:C:H1'     | 2.45                     | 0.51              |
| 8:n:70:VAL:HG13    | 8:n:160:ALA:HB2    | 1.93                     | 0.51              |
| 9:o:39:ARG:HA      | 9:o:42:ILE:HG12    | 1.92                     | 0.51              |
| 15:u:126:LYS:O     | 15:u:129:VAL:HG12  | 2.11                     | 0.51              |
| 45:i:109:GLN:NE2   | 45:i:109:GLN:N     | 2.58                     | 0.51              |
| 45:i:116:GLU:OE1   | 50:F:118:ARG:HG3   | 2.10                     | 0.51              |
| 46:B:415:A:H4'     | 46:B:416:G:O5'     | 2.11                     | 0.51              |
| 46:B:857:G:N2      | 46:B:1032:G:H4'    | 2.26                     | 0.51              |
| 46:B:1516:C:H2'    | 46:B:1517:C:C6     | 2.46                     | 0.51              |
| 79:AR:10:ARG:NH1   | 79:AR:311:GLN:OE1  | 2.44                     | 0.51              |
| 79:AR:155:VAL:O    | 79:AR:156:ARG:NH1  | 2.35                     | 0.51              |
| 1:AS:195:G:N1      | 1:AS:198:A:OP2     | 2.42                     | 0.51              |
| 1:AS:606:A:C5      | 8:BA:21:ARG:HD3    | 2.46                     | 0.51              |
| 1:AS:1587:G:H1'    | 1:AS:1795:A:N1     | 2.26                     | 0.51              |
| 2:AT:94:C:H2'      | 2:AT:95:A:C8       | 2.45                     | 0.51              |
| 16:BI:16:SER:HA    | 37:CD:49:LEU:O     | 2.10                     | 0.51              |
| 20:BM:149:ALA:O    | 20:BM:153:LYS:HG2  | 2.11                     | 0.51              |
| 23:BP:22:PRO:HB3   | 23:BP:96:ILE:HD11  | 1.92                     | 0.51              |
| 46:CM:804:U:H2'    | 46:CM:805:U:H5     | 1.76                     | 0.51              |
| 46:CM:1325:U:O4'   | 46:CM:1364:U:H5''  | 2.10                     | 0.51              |
| 46:CM:1610:C:H2'   | 46:CM:1611:C:H6    | 1.75                     | 0.51              |
| 48:CO:131:ASP:OD2  | 48:CO:133:TYR:CD1  | 2.64                     | 0.51              |
| 51:CR:103:TYR:CD1  | 51:CR:189:LEU:HD21 | 2.46                     | 0.51              |
| 55:CV:78:ILE:HD13  | 55:CV:104:ILE:HG22 | 1.92                     | 0.51              |
| 59:CZ:128:ALA:CB   | 59:CZ:132:GLU:HB2  | 2.40                     | 0.51              |
| 64:DE:93:LEU:HD12  | 64:DE:98:GLY:O     | 2.11                     | 0.51              |
| 79:DT:162:GLN:H    | 79:DT:162:GLN:CD   | 2.17                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:DT:271:LEU:HD12 | 79:DT:310:TRP:CE3  | 2.46                     | 0.51              |
| 1:1:245:G:H1'      | 14:BG:133:SER:OG   | 2.11                     | 0.51              |
| 1:1:277:G:H2'      | 1:1:278:U:C6       | 2.46                     | 0.51              |
| 1:1:1194:C:OP2     | 1:1:1195:C:O2'     | 2.26                     | 0.51              |
| 1:1:1863:A:H2'     | 1:1:1864:G:C8      | 2.46                     | 0.51              |
| 1:1:3234:U:H3      | 8:n:134:ARG:NH1    | 2.09                     | 0.51              |
| 23:5:55:SER:HB2    | 23:5:67:VAL:HB     | 1.92                     | 0.51              |
| 46:B:38:C:O3'      | 56:L:6:ARG:NE      | 2.44                     | 0.51              |
| 46:B:518:A:H2'     | 46:B:519:A:H8      | 1.75                     | 0.51              |
| 46:B:669:G:H2'     | 46:B:671:G:C8      | 2.45                     | 0.51              |
| 46:B:989:U:H3'     | 46:B:990:A:H5''    | 1.92                     | 0.51              |
| 53:I:1:MET:HE2     | 53:I:106:LEU:O     | 2.10                     | 0.51              |
| 65:U:4:VAL:HG12    | 72:b:78:VAL:HG23   | 1.93                     | 0.51              |
| 1:AS:417:A:H2'     | 1:AS:418:A:C8      | 2.46                     | 0.51              |
| 1:AS:631:U:H2'     | 1:AS:632:C:C6      | 2.46                     | 0.51              |
| 1:AS:647:A:H2'     | 1:AS:648:C:C6      | 2.46                     | 0.51              |
| 1:AS:1516:G:H2'    | 1:AS:1517:G:O4'    | 2.10                     | 0.51              |
| 1:AS:2956:C:H2'    | 1:AS:2957:C:H6     | 1.76                     | 0.51              |
| 7:AZ:95:TRP:CE3    | 7:AZ:198:TYR:HB3   | 2.46                     | 0.51              |
| 10:BC:173:LYS:NZ   | 37:CD:45:GLU:OE1   | 2.33                     | 0.51              |
| 14:BG:198:GLU:HB2  | 14:BG:201:LYS:HD2  | 1.93                     | 0.51              |
| 24:BQ:36:VAL:HG22  | 24:BQ:58:VAL:HG11  | 1.93                     | 0.51              |
| 45:CL:107:TRP:CZ3  | 50:CQ:143:LEU:HD12 | 2.46                     | 0.51              |
| 46:CM:157:U:H5'    | 71:DL:117:LYS:HB3  | 1.92                     | 0.51              |
| 46:CM:188:U:H2'    | 46:CM:189:G:H8     | 1.75                     | 0.51              |
| 46:CM:978:A:O3'    | 46:CM:1765:G:H4'   | 2.11                     | 0.51              |
| 46:CM:1776:G:OP2   | 61:DB:127:ARG:NH2  | 2.30                     | 0.51              |
| 48:CO:87:ARG:HH21  | 48:CO:99:ASN:ND2   | 2.09                     | 0.51              |
| 52:CS:210:ALA:O    | 52:CS:214:LYS:N    | 2.33                     | 0.51              |
| 54:CU:30:LEU:HD23  | 54:CU:30:LEU:H     | 1.76                     | 0.51              |
| 59:CZ:40:GLY:C     | 59:CZ:124:LYS:H    | 2.18                     | 0.51              |
| 64:DE:7:LYS:O      | 64:DE:11:ARG:HG2   | 2.11                     | 0.51              |
| 65:DF:91:ASP:OD1   | 65:DF:92:GLN:N     | 2.43                     | 0.51              |
| 81:P0:14:LYS:H     | 81:P0:14:LYS:HD2   | 1.76                     | 0.51              |
| 1:1:169:G:N2       | 1:1:249:G:O3'      | 2.44                     | 0.51              |
| 1:1:182:G:H4'      | 3:4:68:A:O2'       | 2.10                     | 0.51              |
| 1:1:185:U:H3       | 1:1:229:C:N4       | 2.03                     | 0.51              |
| 1:1:1358:C:H2'     | 1:1:1359:A:C8      | 2.46                     | 0.51              |
| 1:1:2239:G:O2'     | 1:1:2241:C:N4      | 2.44                     | 0.51              |
| 1:1:2444:G:N2      | 1:1:2467:C:O2'     | 2.44                     | 0.51              |
| 23:5:16:VAL:HG12   | 23:5:65:VAL:HG22   | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:AE:11:TYR:O     | 32:AE:71:ARG:HD2   | 2.11                     | 0.51              |
| 46:B:211:A:H62     | 46:B:250:U:H3      | 1.57                     | 0.51              |
| 46:B:222:C:N4      | 46:B:823:G:H21     | 2.08                     | 0.51              |
| 46:B:801:A:O4'     | 54:J:106:GLN:NE2   | 2.44                     | 0.51              |
| 46:B:1048:U:O2'    | 48:D:203:THR:OG1   | 2.27                     | 0.51              |
| 46:B:1609:G:H2'    | 46:B:1610:C:C6     | 2.46                     | 0.51              |
| 47:C:59:LEU:HD22   | 68:X:79:LEU:HD11   | 1.93                     | 0.51              |
| 50:F:109:LYS:HE3   | 50:F:114:LEU:HD22  | 1.93                     | 0.51              |
| 57:M:77:ARG:NE     | 57:M:86:ILE:HG22   | 2.25                     | 0.51              |
| 1:AS:449:U:H2'     | 1:AS:450:G:H8      | 1.75                     | 0.51              |
| 1:AS:656:G:N2      | 6:AY:94:MET:HB2    | 2.26                     | 0.51              |
| 1:AS:687:U:O4      | 6:AY:210:TYR:OH    | 2.24                     | 0.51              |
| 1:AS:1046:U:OP2    | 22:BO:13:TYR:OH    | 2.25                     | 0.51              |
| 1:AS:1705:C:H2'    | 1:AS:1706:C:H6     | 1.74                     | 0.51              |
| 83:AS:3401:3K5:H16 | 83:AS:3401:3K5:H39 | 1.92                     | 0.51              |
| 2:AT:70:A:H2'      | 2:AT:71:U:C6       | 2.45                     | 0.51              |
| 4:AW:66:PRO:HG2    | 4:AW:67:TYR:CE2    | 2.46                     | 0.51              |
| 6:AY:113:LYS:HG2   | 16:BI:202:TYR:HB3  | 1.93                     | 0.51              |
| 21:BN:71:LYS:O     | 21:BN:73:LYS:NZ    | 2.38                     | 0.51              |
| 21:BN:99:ARG:NH1   | 21:BN:126:VAL:O    | 2.35                     | 0.51              |
| 26:BS:91:ASN:OD1   | 26:BS:93:HIS:N     | 2.43                     | 0.51              |
| 28:BU:53:VAL:CG1   | 28:BU:62:VAL:HG13  | 2.41                     | 0.51              |
| 46:CM:871:U:O2'    | 61:DB:116:VAL:O    | 2.29                     | 0.51              |
| 46:CM:1026:G:H2'   | 46:CM:1027:G:H8    | 1.73                     | 0.51              |
| 62:DC:64:ARG:NH1   | 62:DC:92:SER:OG    | 2.44                     | 0.51              |
| 66:DG:42:GLY:HA2   | 66:DG:84:LYS:HG3   | 1.92                     | 0.51              |
| 1:1:152:U:H4'      | 1:1:157:G:H4'      | 1.94                     | 0.50              |
| 1:1:169:G:N1       | 1:1:249:G:H1'      | 2.26                     | 0.50              |
| 1:1:2322:U:H2'     | 1:1:2323:A:H8      | 1.75                     | 0.50              |
| 1:1:2876:U:H2'     | 1:1:2877:U:C6      | 2.45                     | 0.50              |
| 6:l:301:ARG:NH2    | 19:y:38:ARG:O      | 2.44                     | 0.50              |
| 9:o:52:GLU:OE2     | 9:o:184:HIS:NE2    | 2.44                     | 0.50              |
| 10:p:42:GLN:OE1    | 10:p:45:ARG:NH2    | 2.43                     | 0.50              |
| 15:u:52:LEU:HD23   | 15:u:55:ILE:HD11   | 1.91                     | 0.50              |
| 27:9:11:SER:HB3    | 27:9:14:LYS:HB2    | 1.93                     | 0.50              |
| 46:B:874:U:H2'     | 46:B:875:C:C6      | 2.45                     | 0.50              |
| 46:B:1143:C:O2'    | 46:B:1568:C:OP2    | 2.29                     | 0.50              |
| 46:B:1440:G:O2'    | 62:R:122:THR:OG1   | 2.17                     | 0.50              |
| 46:B:1672:G:N2     | 46:B:1704:C:C2     | 2.79                     | 0.50              |
| 57:M:54:TYR:CD1    | 57:M:72:GLY:HA2    | 2.45                     | 0.50              |
| 1:AS:716:G:H3'     | 1:AS:717:A:H5''    | 1.92                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:788:G:H2'     | 1:AS:789:C:H6      | 1.73                     | 0.50              |
| 1:AS:1099:A:N6     | 1:AS:1359:A:N3     | 2.53                     | 0.50              |
| 1:AS:3093:U:H1'    | 1:AS:3094:A:H5''   | 1.94                     | 0.50              |
| 5:AX:159:ARG:HG2   | 5:AX:182:GLN:HA    | 1.93                     | 0.50              |
| 11:BD:47:LYS:HE3   | 11:BD:49:ASN:C     | 2.37                     | 0.50              |
| 28:BU:83:THR:HB    | 28:BU:85:TYR:HD1   | 1.74                     | 0.50              |
| 46:CM:137:A:O4'    | 46:CM:139:U:H5'    | 2.11                     | 0.50              |
| 46:CM:379:C:OP1    | 51:CR:10:LYS:NZ    | 2.37                     | 0.50              |
| 46:CM:1351:U:P     | 63:DD:65:ARG:HH21  | 2.34                     | 0.50              |
| 46:CM:1469:A:H2'   | 46:CM:1470:G:C8    | 2.46                     | 0.50              |
| 50:CQ:60:LEU:HD11  | 50:CQ:89:ALA:HB3   | 1.92                     | 0.50              |
| 54:CU:29:ASP:OD1   | 54:CU:29:ASP:N     | 2.44                     | 0.50              |
| 54:CU:139:LEU:HB2  | 54:CU:143:ASN:O    | 2.11                     | 0.50              |
| 73:DN:11:ASN:HB3   | 73:DN:33:ASP:HB2   | 1.92                     | 0.50              |
| 79:DT:148:HIS:HE2  | 79:DT:176:LYS:HB2  | 1.76                     | 0.50              |
| 79:DT:262:LEU:HD23 | 79:DT:263:GLN:H    | 1.75                     | 0.50              |
| 1:1:1235:C:C2      | 1:1:1236:A:C8      | 2.99                     | 0.50              |
| 1:1:1705:C:H2'     | 1:1:1706:C:H6      | 1.77                     | 0.50              |
| 1:1:2439:A:OP2     | 1:1:2439:A:H8      | 1.95                     | 0.50              |
| 1:1:3256:G:H2'     | 1:1:3257:A:C8      | 2.45                     | 0.50              |
| 45:i:107:TRP:CZ2   | 50:F:143:LEU:HD13  | 2.46                     | 0.50              |
| 46:B:261:C:O2'     | 46:B:262:G:H5'     | 2.12                     | 0.50              |
| 46:B:560:G:H2'     | 46:B:561:U:O2      | 2.11                     | 0.50              |
| 46:B:1573:A:H2'    | 46:B:1574:A:O4'    | 2.11                     | 0.50              |
| 52:H:42:LEU:HB3    | 52:H:46:TRP:HB2    | 1.94                     | 0.50              |
| 54:J:8:GLU:H       | 54:J:8:GLU:CD      | 2.19                     | 0.50              |
| 58:N:26:LYS:NZ     | 58:N:29:LYS:HD2    | 2.25                     | 0.50              |
| 58:N:66:ILE:HD13   | 58:N:128:CYS:HB3   | 1.93                     | 0.50              |
| 64:T:17:ILE:HB     | 64:T:69:ILE:HD12   | 1.92                     | 0.50              |
| 1:AS:25:A:H2'      | 1:AS:26:C:H6       | 1.75                     | 0.50              |
| 1:AS:273:A:H1'     | 37:CD:77:GLY:HA3   | 1.93                     | 0.50              |
| 1:AS:2206:A:H2'    | 1:AS:2207:A:H8     | 1.74                     | 0.50              |
| 1:AS:3256:G:H2'    | 1:AS:3257:A:C8     | 2.46                     | 0.50              |
| 1:AS:3285:A:H2'    | 1:AS:3286:C:C6     | 2.47                     | 0.50              |
| 10:BC:74:PRO:HD3   | 10:BC:234:TRP:CD2  | 2.47                     | 0.50              |
| 13:BF:82:ARG:HH22  | 13:BF:114:ILE:HD11 | 1.75                     | 0.50              |
| 27:BT:31:LEU:HB3   | 27:BT:101:PRO:HG2  | 1.93                     | 0.50              |
| 46:CM:309:U:OP2    | 70:DK:20:ARG:HD3   | 2.11                     | 0.50              |
| 46:CM:488:C:C2     | 46:CM:495:G:N2     | 2.79                     | 0.50              |
| 46:CM:870:G:N2     | 61:DB:118:SER:O    | 2.42                     | 0.50              |
| 46:CM:1446:A:H5''  | 62:DC:128:HIS:HE1  | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1484:U:O4'   | 46:CM:1506:U:H4'   | 2.11                     | 0.50              |
| 55:CV:37:LYS:NZ    | 55:CV:93:THR:HB    | 2.25                     | 0.50              |
| 79:DT:7:LEU:O      | 79:DT:310:TRP:HE3  | 1.94                     | 0.50              |
| 82:12:143:VAL:HG11 | 82:12:148:PRO:HG3  | 1.91                     | 0.50              |
| 1:1:208:A:H4'      | 1:1:210:A:N7       | 2.26                     | 0.50              |
| 1:1:511:C:H5''     | 6:l:344:LYS:HD2    | 1.93                     | 0.50              |
| 1:1:699:G:H2'      | 1:1:700:C:C6       | 2.45                     | 0.50              |
| 1:1:1493:C:H2'     | 1:1:1494:A:H8      | 1.76                     | 0.50              |
| 1:1:1754:G:H2'     | 1:1:1755:U:O4'     | 2.11                     | 0.50              |
| 1:1:1911:A:H2'     | 1:1:1912:U:C6      | 2.47                     | 0.50              |
| 1:1:2872:A:H5'     | 41:AN:51:LEU:HD21  | 1.93                     | 0.50              |
| 7:m:286:VAL:HG13   | 12:r:206:LEU:HD22  | 1.93                     | 0.50              |
| 9:o:105:ARG:NH2    | 9:o:197:SER:O      | 2.44                     | 0.50              |
| 16:v:113:LEU:HB2   | 16:v:134:LEU:HD23  | 1.93                     | 0.50              |
| 20:z:177:LEU:HA    | 20:z:180:LYS:HD2   | 1.94                     | 0.50              |
| 35:AH:9:ARG:HD2    | 35:AH:34:HIS:ND1   | 2.26                     | 0.50              |
| 46:B:623:C:H2'     | 46:B:624:U:C6      | 2.47                     | 0.50              |
| 46:B:770:C:H6      | 46:B:770:C:OP1     | 1.93                     | 0.50              |
| 46:B:1102:U:H2'    | 46:B:1103:G:C8     | 2.46                     | 0.50              |
| 46:B:1219:A:O2'    | 78:h:182:TYR:OH    | 2.21                     | 0.50              |
| 47:C:147:THR:CG2   | 47:C:159:ALA:HB1   | 2.42                     | 0.50              |
| 58:N:125:VAL:HG12  | 58:N:139:VAL:HA    | 1.93                     | 0.50              |
| 1:AS:565:A:H2'     | 1:AS:566:C:O4'     | 2.11                     | 0.50              |
| 1:AS:2145:A:H2'    | 1:AS:2146:A:C8     | 2.46                     | 0.50              |
| 3:AU:21:C:OP1      | 6:AY:194:LYS:NZ    | 2.29                     | 0.50              |
| 11:BD:80:THR:HA    | 11:BD:83:THR:HG22  | 1.93                     | 0.50              |
| 23:BP:37:LEU:HD12  | 23:BP:56:ILE:HG21  | 1.93                     | 0.50              |
| 28:BU:46:ILE:HG23  | 28:BU:68:VAL:HG13  | 1.94                     | 0.50              |
| 31:BX:60:TYR:OH    | 35:CB:97:GLU:OE2   | 2.28                     | 0.50              |
| 32:BY:78:ARG:HA    | 32:BY:88:LEU:HD23  | 1.93                     | 0.50              |
| 46:CM:565:A:N3     | 77:DR:14:VAL:HG21  | 2.25                     | 0.50              |
| 46:CM:933:A:H2'    | 46:CM:934:C:H6     | 1.76                     | 0.50              |
| 46:CM:940:A:H4'    | 46:CM:1058:G:O2'   | 2.11                     | 0.50              |
| 46:CM:1518:G:H21   | 66:DG:48:GLN:CD    | 2.19                     | 0.50              |
| 50:CQ:215:GLU:CG   | 50:CQ:216:ASP:H    | 2.21                     | 0.50              |
| 54:CU:169:TYR:CE1  | 54:CU:173:THR:HG21 | 2.46                     | 0.50              |
| 64:DE:93:LEU:HD23  | 64:DE:93:LEU:H     | 1.76                     | 0.50              |
| 65:DF:16:ARG:NH1   | 65:DF:21:ASN:OD1   | 2.44                     | 0.50              |
| 74:DO:64:CYS:HB3   | 74:DO:73:LEU:HD23  | 1.93                     | 0.50              |
| 79:DT:84:ALA:HB2   | 79:DT:114:VAL:HB   | 1.94                     | 0.50              |
| 1:1:690:A:O4'      | 6:l:47:LYS:HG3     | 2.11                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1:1089:A:OP2     | 22:2:120:LYS:NZ   | 2.35                     | 0.50              |
| 1:1:1140:U:OP1     | 1:1:1363:G:O2'    | 2.25                     | 0.50              |
| 1:1:2079:C:OP1     | 20:z:71:ARG:NH1   | 2.44                     | 0.50              |
| 1:1:2442:U:H4'     | 1:1:2443:G:OP2    | 2.12                     | 0.50              |
| 1:1:3308:G:H21     | 1:1:3327:A:H2     | 1.59                     | 0.50              |
| 10:p:201:LEU:HD23  | 10:p:203:GLU:H    | 1.76                     | 0.50              |
| 16:v:48:ALA:HA     | 16:v:133:ILE:HD11 | 1.92                     | 0.50              |
| 28:AA:24:VAL:HG21  | 28:AA:87:LEU:HB3  | 1.92                     | 0.50              |
| 45:i:90:ARG:NH2    | 46:B:1624:C:H2'   | 2.26                     | 0.50              |
| 46:B:871:U:C2      | 46:B:872:A:C8     | 3.00                     | 0.50              |
| 46:B:933:A:H2'     | 46:B:934:C:C6     | 2.47                     | 0.50              |
| 46:B:1664:C:H42    | 46:B:1711:C:H42   | 1.59                     | 0.50              |
| 1:AS:180:U:H4'     | 38:CE:75:LYS:CG   | 2.42                     | 0.50              |
| 1:AS:1198:A:C2     | 1:AS:2829:C:H5'   | 2.47                     | 0.50              |
| 1:AS:2183:U:O2'    | 1:AS:2184:G:OP1   | 2.25                     | 0.50              |
| 1:AS:2967:A:H2'    | 1:AS:2968:U:O4'   | 2.12                     | 0.50              |
| 1:AS:3216:U:H2'    | 1:AS:3217:G:C8    | 2.46                     | 0.50              |
| 2:AT:35:C:O2       | 2:AT:45:A:O2'     | 2.29                     | 0.50              |
| 20:BM:20:ARG:NH1   | 20:BM:21:LYS:HZ2  | 2.10                     | 0.50              |
| 27:BT:11:SER:HB3   | 27:BT:14:LYS:HB2  | 1.93                     | 0.50              |
| 28:BU:58:ASP:O     | 28:BU:62:VAL:HG23 | 2.11                     | 0.50              |
| 36:CC:19:SER:O     | 36:CC:23:GLU:HG3  | 2.11                     | 0.50              |
| 46:CM:1212:A:C2    | 59:CZ:43:ARG:HB2  | 2.47                     | 0.50              |
| 46:CM:1242:U:H2'   | 46:CM:1242:U:O2   | 2.11                     | 0.50              |
| 78:DS:165:ALA:C    | 78:DS:167:THR:H   | 2.20                     | 0.50              |
| 78:DS:168:CYS:HB3  | 78:DS:185:LYS:HB3 | 1.94                     | 0.50              |
| 79:DT:10:ARG:NH2   | 79:DT:50:GLY:O    | 2.44                     | 0.50              |
| 79:DT:62:PHE:HB3   | 79:DT:93:TRP:CE3  | 2.47                     | 0.50              |
| 79:DT:217:ILE:HD11 | 79:DT:233:ALA:HB2 | 1.93                     | 0.50              |
| 1:1:941:C:H2'      | 1:1:942:U:H6      | 1.76                     | 0.50              |
| 1:1:1012:U:H3'     | 1:1:1013:U:O3'    | 2.12                     | 0.50              |
| 1:1:1714:G:H2'     | 1:1:1715:G:H8     | 1.76                     | 0.50              |
| 1:1:2331:G:H5''    | 18:x:86:LYS:HB2   | 1.93                     | 0.50              |
| 1:1:2853:C:H2'     | 1:1:2854:U:C6     | 2.46                     | 0.50              |
| 7:m:19:PRO:HG2     | 7:m:24:GLN:HB2    | 1.94                     | 0.50              |
| 11:q:89:LYS:HB2    | 11:q:183:GLU:HB3  | 1.93                     | 0.50              |
| 46:B:291:U:H2'     | 46:B:292:C:H6     | 1.77                     | 0.50              |
| 46:B:339:A:H2'     | 46:B:340:C:C6     | 2.46                     | 0.50              |
| 46:B:511:U:O4      | 56:L:171:ARG:NH2  | 2.45                     | 0.50              |
| 46:B:637:U:N3      | 54:J:96:PRO:HA    | 2.25                     | 0.50              |
| 50:F:172:ALA:HB1   | 50:F:174:ARG:NH1  | 2.26                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AS:236:A:OP1    | 3:AU:95:G:N2       | 2.34                     | 0.50              |
| 1:AS:1633:A:H4'   | 28:BU:15:ARG:HD2   | 1.92                     | 0.50              |
| 1:AS:1683:U:H5'   | 23:BP:81:TYR:HE2   | 1.76                     | 0.50              |
| 1:AS:2197:A:H2'   | 1:AS:2198:A:H8     | 1.77                     | 0.50              |
| 1:AS:2251:G:H22   | 1:AS:2290:A:P      | 2.35                     | 0.50              |
| 1:AS:2417:A:H2'   | 1:AS:2418:A:C8     | 2.46                     | 0.50              |
| 1:AS:2417:A:H2'   | 1:AS:2418:A:H8     | 1.77                     | 0.50              |
| 19:BL:44:PHE:CD2  | 19:BL:134:GLY:HA3  | 2.47                     | 0.50              |
| 22:BO:118:GLU:O   | 22:BO:122:ASN:N    | 2.39                     | 0.50              |
| 45:CL:108:GLY:HA3 | 50:CQ:117:ARG:HG2  | 1.93                     | 0.50              |
| 52:CS:30:PRO:HB2  | 52:CS:32:ASP:OD1   | 2.11                     | 0.50              |
| 54:CU:59:PRO:O    | 54:CU:62:SER:OG    | 2.23                     | 0.50              |
| 54:CU:155:SER:O   | 54:CU:157:ALA:N    | 2.43                     | 0.50              |
| 54:CU:173:THR:HB  | 54:CU:175:LYS:NZ   | 2.26                     | 0.50              |
| 79:DT:16:HIS:HE1  | 79:DT:37:SER:CB    | 2.24                     | 0.50              |
| 79:DT:258:LYS:HG3 | 79:DT:267:LEU:HD13 | 1.93                     | 0.50              |
| 1:1:634:C:O2      | 1:1:2355:G:O2'     | 2.21                     | 0.50              |
| 1:1:956:U:H4'     | 1:1:959:G:N1       | 2.26                     | 0.50              |
| 1:1:1593:C:H2'    | 1:1:1594:G:H8      | 1.76                     | 0.50              |
| 1:1:2974:C:OP1    | 5:k:26:ARG:NH1     | 2.44                     | 0.50              |
| 13:s:47:GLN:OE1   | 13:s:64:LYS:HD3    | 2.12                     | 0.50              |
| 17:w:122:PRO:HA   | 17:w:125:LEU:HD12  | 1.93                     | 0.50              |
| 20:z:39:SER:HA    | 20:z:42:ARG:HH11   | 1.77                     | 0.50              |
| 23:5:51:GLY:O     | 23:5:53:ASP:N      | 2.36                     | 0.50              |
| 25:7:96:GLN:O     | 25:7:97:LYS:HB3    | 2.12                     | 0.50              |
| 46:B:282:G:N7     | 53:I:188:ARG:NH2   | 2.55                     | 0.50              |
| 46:B:415:A:H5'    | 46:B:416:G:C5      | 2.45                     | 0.50              |
| 46:B:872:A:H1'    | 61:Q:117:PRO:HB3   | 1.93                     | 0.50              |
| 46:B:944:U:H5'    | 60:P:15:ALA:O      | 2.12                     | 0.50              |
| 46:B:1659:G:H2'   | 46:B:1660:G:H8     | 1.76                     | 0.50              |
| 49:E:133:PRO:HB2  | 49:E:217:TYR:HE2   | 1.75                     | 0.50              |
| 51:G:139:VAL:HG23 | 51:G:150:PRO:HG3   | 1.93                     | 0.50              |
| 52:H:25:LEU:HD22  | 63:S:56:LEU:HD22   | 1.94                     | 0.50              |
| 76:f:33:LYS:HE2   | 76:f:34:TYR:CZ     | 2.46                     | 0.50              |
| 1:AS:371:G:N1     | 1:AS:374:A:OP2     | 2.40                     | 0.50              |
| 1:AS:561:U:H2'    | 1:AS:562:C:C6      | 2.47                     | 0.50              |
| 1:AS:1718:U:H5''  | 20:BM:99:LEU:HD23  | 1.94                     | 0.50              |
| 1:AS:1863:A:H2'   | 1:AS:1864:G:H8     | 1.77                     | 0.50              |
| 1:AS:1869:U:OP1   | 20:BM:21:LYS:NZ    | 2.45                     | 0.50              |
| 1:AS:2594:C:N4    | 80:BE:116:ARG:HH12 | 2.09                     | 0.50              |
| 14:BG:51:ILE:HG13 | 14:BG:52:ASP:N     | 2.26                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:BK:29:THR:HG22  | 18:BK:119:VAL:HG21 | 1.93                     | 0.50              |
| 28:BU:25:ILE:HA    | 28:BU:43:VAL:HG12  | 1.94                     | 0.50              |
| 46:CM:810:U:H2'    | 46:CM:811:U:O4'    | 2.12                     | 0.50              |
| 46:CM:1498:G:H2'   | 46:CM:1499:G:C8    | 2.47                     | 0.50              |
| 46:CM:1762:U:H2'   | 46:CM:1763:A:C8    | 2.47                     | 0.50              |
| 52:CS:164:PRO:HD3  | 75:DP:54:LEU:HD23  | 1.94                     | 0.50              |
| 53:CT:142:ARG:HG2  | 53:CT:147:LEU:HD12 | 1.93                     | 0.50              |
| 59:CZ:51:ALA:HB1   | 59:CZ:122:VAL:HG11 | 1.92                     | 0.50              |
| 62:DC:64:ARG:HH12  | 62:DC:92:SER:N     | 2.10                     | 0.50              |
| 78:DS:183:CYS:HB3  | 78:DS:188:LEU:CD2  | 2.41                     | 0.50              |
| 79:DT:112:LEU:HD11 | 79:DT:128:ARG:HG3  | 1.94                     | 0.50              |
| 1:1:259:C:H2'      | 1:1:260:C:C6       | 2.47                     | 0.50              |
| 1:1:381:U:H2'      | 1:1:382:U:C6       | 2.47                     | 0.50              |
| 1:1:510:G:N2       | 6:l:341:GLY:O      | 2.45                     | 0.50              |
| 1:1:538:G:O2'      | 1:1:539:G:OP1      | 2.28                     | 0.50              |
| 1:1:1151:C:H2'     | 1:1:1152:C:C6      | 2.47                     | 0.50              |
| 1:1:2873:G:O2'     | 1:1:2996:A:N1      | 2.45                     | 0.50              |
| 1:1:3066:A:H2'     | 1:1:3067:U:C6      | 2.47                     | 0.50              |
| 3:4:113:U:H5''     | 40:AM:7:PHE:HB2    | 1.93                     | 0.50              |
| 6:l:318:PRO:O      | 6:l:325:LEU:HB2    | 2.11                     | 0.50              |
| 21:0:73:LYS:NZ     | 21:0:97:VAL:O      | 2.42                     | 0.50              |
| 25:7:60:LYS:HA     | 25:7:63:ILE:HD12   | 1.94                     | 0.50              |
| 32:AE:61:ARG:HB2   | 32:AE:65:GLY:HA3   | 1.94                     | 0.50              |
| 46:B:415:A:H5'     | 46:B:416:G:C4      | 2.47                     | 0.50              |
| 46:B:978:A:O3'     | 46:B:1765:G:H4'    | 2.12                     | 0.50              |
| 46:B:1608:U:H2'    | 46:B:1609:G:C8     | 2.47                     | 0.50              |
| 47:C:79:ARG:O      | 47:C:83:GLN:HG3    | 2.12                     | 0.50              |
| 57:M:77:ARG:HD2    | 57:M:84:GLU:HA     | 1.93                     | 0.50              |
| 1:AS:61:A:H2'      | 1:AS:62:A:C8       | 2.47                     | 0.50              |
| 1:AS:907:C:N4      | 4:AW:3:ARG:HD3     | 2.27                     | 0.50              |
| 1:AS:1642:G:H1'    | 1:AS:1805:A:N6     | 2.27                     | 0.50              |
| 1:AS:3005:A:H2'    | 1:AS:3006:C:H6     | 1.77                     | 0.50              |
| 1:AS:3179:U:H4'    | 34:CA:3:GLU:HG2    | 1.94                     | 0.50              |
| 26:BS:121:LYS:HD3  | 26:BS:123:TYR:CZ   | 2.47                     | 0.50              |
| 36:CC:34:GLN:HB3   | 36:CC:38:ARG:HE    | 1.77                     | 0.50              |
| 39:CF:56:VAL:HG21  | 39:CF:65:LEU:CD2   | 2.41                     | 0.50              |
| 46:CM:157:U:O2'    | 53:CT:87:ARG:NE    | 2.44                     | 0.50              |
| 46:CM:530:U:OP1    | 71:DL:64:PHE:HA    | 2.12                     | 0.50              |
| 46:CM:1212:A:H3'   | 59:CZ:117:GLY:O    | 2.12                     | 0.50              |
| 46:CM:1609:G:H2'   | 46:CM:1610:C:C6    | 2.46                     | 0.50              |
| 52:CS:26:ALA:HB2   | 63:DD:25:LYS:CB    | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:CY:56:LYS:HE2  | 58:CY:57:LYS:HE3  | 1.92                     | 0.50              |
| 70:DK:73:ARG:HH21 | 70:DK:82:LYS:HD3  | 1.76                     | 0.50              |
| 79:DT:16:HIS:CD2  | 79:DT:20:VAL:HG13 | 2.46                     | 0.50              |
| 79:DT:195:TYR:CE2 | 79:DT:213:LYS:HD2 | 2.45                     | 0.50              |
| 79:DT:286:ALA:HA  | 79:DT:302:TYR:HA  | 1.91                     | 0.50              |
| 1:1:429:U:H2'     | 1:1:430:G:C8      | 2.41                     | 0.50              |
| 1:1:2138:G:H2'    | 1:1:2139:G:C8     | 2.45                     | 0.50              |
| 1:1:2354:G:H2'    | 1:1:2355:G:C8     | 2.46                     | 0.50              |
| 1:1:2385:C:H2'    | 1:1:2386:U:C6     | 2.47                     | 0.50              |
| 1:1:3194:G:H5'    | 15:u:129:VAL:HG21 | 1.93                     | 0.50              |
| 1:1:3300:A:H2'    | 1:1:3301:A:C8     | 2.46                     | 0.50              |
| 83:1:3401:3K5:H30 | 43:AP:40:LYS:HD3  | 1.94                     | 0.50              |
| 3:4:155:G:H5'     | 10:p:186:ARG:HD2  | 1.92                     | 0.50              |
| 29:AB:73:ILE:HB   | 29:AB:109:TYR:CD2 | 2.47                     | 0.50              |
| 46:B:840:A:O2'    | 46:B:841:A:H3'    | 2.12                     | 0.50              |
| 46:B:1259:C:O2    | 46:B:1413:A:O2'   | 2.28                     | 0.50              |
| 46:B:1306:A:H4'   | 46:B:1307:A:O5'   | 2.11                     | 0.50              |
| 47:C:53:THR:OG1   | 47:C:161:PRO:HG2  | 2.11                     | 0.50              |
| 62:R:130:ARG:O    | 62:R:130:ARG:HG2  | 2.11                     | 0.50              |
| 65:U:29:MET:HB2   | 65:U:54:LEU:HD22  | 1.93                     | 0.50              |
| 1:AS:120:A:C2     | 10:BC:130:PRO:HB3 | 2.46                     | 0.50              |
| 1:AS:289:A:H2'    | 1:AS:290:G:C8     | 2.45                     | 0.50              |
| 1:AS:292:U:P      | 16:BI:68:ARG:HH22 | 2.35                     | 0.50              |
| 1:AS:421:G:O6     | 1:AS:2361:C:O2'   | 2.23                     | 0.50              |
| 1:AS:1911:A:H2'   | 1:AS:1912:U:C6    | 2.47                     | 0.50              |
| 3:AU:75:G:OP2     | 27:BT:74:TYR:OH   | 2.30                     | 0.50              |
| 24:BQ:23:MET:HE1  | 24:BQ:78:VAL:HG22 | 1.94                     | 0.50              |
| 46:CM:122:U:C2'   | 46:CM:123:G:H5''  | 2.42                     | 0.50              |
| 46:CM:857:G:H2'   | 46:CM:858:U:O4'   | 2.12                     | 0.50              |
| 46:CM:1332:U:C5   | 67:DH:57:MET:HE1  | 2.47                     | 0.50              |
| 46:CM:1567:C:H4'  | 63:DD:136:ARG:HB2 | 1.94                     | 0.50              |
| 46:CM:1628:C:H2'  | 46:CM:1629:G:C8   | 2.47                     | 0.50              |
| 46:CM:1672:G:C2'  | 46:CM:1673:U:H5'  | 2.42                     | 0.50              |
| 54:CU:85:HIS:CE1  | 54:CU:160:TYR:HD2 | 2.30                     | 0.50              |
| 59:CZ:59:LEU:HA   | 59:CZ:87:PRO:O    | 2.11                     | 0.50              |
| 79:DT:202:SER:OG  | 79:DT:207:LEU:HB2 | 2.11                     | 0.50              |
| 79:DT:259:ILE:HB  | 79:DT:268:LEU:H   | 1.77                     | 0.50              |
| 1:1:127:G:OP1     | 36:AI:75:TYR:OH   | 2.23                     | 0.50              |
| 1:1:285:A:O2'     | 43:AP:45:ARG:NH1  | 2.36                     | 0.50              |
| 1:1:289:A:H2'     | 1:1:290:G:C8      | 2.45                     | 0.50              |
| 1:1:827:G:O2'     | 1:1:1860:A:N3     | 2.41                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:2089:G:O2'    | 25:7:44:LYS:NZ     | 2.42                     | 0.50              |
| 1:1:2339:A:H2'    | 1:1:2340:C:H6      | 1.77                     | 0.50              |
| 1:1:2473:C:H2'    | 1:1:2474:C:O4'     | 2.12                     | 0.50              |
| 1:1:3025:G:H2'    | 1:1:3026:U:H6      | 1.77                     | 0.50              |
| 1:1:3313:G:N2     | 1:1:3322:U:O2      | 2.34                     | 0.50              |
| 45:i:92:SER:HA    | 46:B:1259:C:C5     | 2.46                     | 0.50              |
| 46:B:335:G:O2'    | 55:K:10:LYS:NZ     | 2.43                     | 0.50              |
| 46:B:521:G:H5'    | 71:a:60:PHE:O      | 2.12                     | 0.50              |
| 51:G:122:LYS:HG2  | 51:G:162:ILE:HB    | 1.92                     | 0.50              |
| 54:J:51:LYS:HD2   | 54:J:85:HIS:CE1    | 2.47                     | 0.50              |
| 59:O:74:LEU:O     | 59:O:78:LEU:HD13   | 2.12                     | 0.50              |
| 63:S:93:GLN:NE2   | 79:AR:61:SER:O     | 2.44                     | 0.50              |
| 1:AS:1380:U:O5'   | 6:AY:203:ARG:HD3   | 2.12                     | 0.50              |
| 1:AS:1655:U:H2'   | 1:AS:1656:C:H6     | 1.77                     | 0.50              |
| 1:AS:1937:C:OP2   | 20:BM:74:ARG:HB3   | 2.12                     | 0.50              |
| 1:AS:3269:C:O3'   | 5:AX:334:ARG:NH2   | 2.45                     | 0.50              |
| 1:AS:3310:G:OP1   | 55:CV:92:ARG:HG3   | 2.11                     | 0.50              |
| 3:AU:56:G:H2'     | 3:AU:57:C:O4'      | 2.11                     | 0.50              |
| 13:BF:62:ASN:C    | 43:CJ:103:ALA:HB2  | 2.37                     | 0.50              |
| 17:BJ:160:LYS:O   | 17:BJ:163:VAL:HG12 | 2.12                     | 0.50              |
| 26:BS:37:THR:OG1  | 26:BS:38:LEU:N     | 2.41                     | 0.50              |
| 46:CM:913:U:H2'   | 46:CM:930:U:OP2    | 2.11                     | 0.50              |
| 46:CM:1155:G:C2   | 46:CM:1156:A:C8    | 2.99                     | 0.50              |
| 46:CM:1431:G:N2   | 78:DS:129:THR:O    | 2.44                     | 0.50              |
| 47:CN:11:PRO:O    | 47:CN:15:LYS:HG3   | 2.12                     | 0.50              |
| 54:CU:67:ARG:CZ   | 54:CU:70:GLN:HG3   | 2.42                     | 0.50              |
| 57:CX:28:ASN:HD21 | 76:DQ:7:TRP:HE1    | 1.60                     | 0.50              |
| 60:DA:45:LEU:HD22 | 60:DA:49:GLN:CD    | 2.37                     | 0.50              |
| 76:DQ:23:HIS:HB2  | 76:DQ:42:CYS:SG    | 2.51                     | 0.50              |
| 1:1:409:A:N1      | 1:1:1437:G:O2'     | 2.37                     | 0.49              |
| 1:1:849:G:OP2     | 44:AQ:2:THR:HG21   | 2.12                     | 0.49              |
| 1:1:922:A:H2'     | 1:1:923:C:C6       | 2.47                     | 0.49              |
| 1:1:1024:U:C2     | 1:1:1025:G:N7      | 2.80                     | 0.49              |
| 1:1:1562:G:C4     | 1:1:1563:A:H1'     | 2.46                     | 0.49              |
| 1:1:1908:U:O2'    | 1:1:2099:G:N7      | 2.39                     | 0.49              |
| 1:1:2379:A:O3'    | 6:l:69:GLY:HA2     | 2.12                     | 0.49              |
| 1:1:2653:U:O2     | 13:s:20:ASN:ND2    | 2.45                     | 0.49              |
| 3:4:75:G:H2'      | 3:4:76:C:C6        | 2.46                     | 0.49              |
| 10:p:79:PHE:HA    | 10:p:180:ILE:HD13  | 1.93                     | 0.49              |
| 25:7:90:ILE:HG22  | 25:7:94:ARG:HD2    | 1.93                     | 0.49              |
| 46:B:291:U:H2'    | 46:B:292:C:C6      | 2.47                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:B:302:U:H2'     | 46:B:303:C:H6     | 1.76                     | 0.49              |
| 49:E:173:ILE:HG21  | 49:E:180:LYS:HA   | 1.94                     | 0.49              |
| 55:K:124:LYS:HB3   | 55:K:129:HIS:ND1  | 2.27                     | 0.49              |
| 1:AS:28:C:OP1      | 16:BI:189:HIS:HB2 | 2.11                     | 0.49              |
| 1:AS:246:U:H2'     | 1:AS:247:C:C6     | 2.46                     | 0.49              |
| 1:AS:270:U:H2'     | 1:AS:271:C:H6     | 1.77                     | 0.49              |
| 1:AS:964:G:H2'     | 1:AS:965:C:C6     | 2.47                     | 0.49              |
| 1:AS:981:U:H2'     | 1:AS:982:U:H6     | 1.76                     | 0.49              |
| 1:AS:1104:U:H2'    | 1:AS:1105:U:H6    | 1.74                     | 0.49              |
| 1:AS:2330:A:H5''   | 18:BK:83:TRP:O    | 2.12                     | 0.49              |
| 1:AS:3134:C:H2'    | 1:AS:3135:A:H8    | 1.76                     | 0.49              |
| 6:AY:260:ASP:OD1   | 6:AY:265:SER:HB3  | 2.12                     | 0.49              |
| 19:BL:123:THR:OG1  | 19:BL:125:ASP:OD1 | 2.27                     | 0.49              |
| 20:BM:38:ARG:O     | 20:BM:42:ARG:HG3  | 2.12                     | 0.49              |
| 23:BP:15:PHE:HB2   | 23:BP:66:VAL:HB   | 1.94                     | 0.49              |
| 25:BR:102:LYS:CD   | 25:BR:105:ARG:NH2 | 2.75                     | 0.49              |
| 28:BU:50:PRO:HD3   | 28:BU:68:VAL:HG22 | 1.93                     | 0.49              |
| 46:CM:57:G:OP2     | 71:DL:116:LYS:HD3 | 2.12                     | 0.49              |
| 46:CM:391:C:H2'    | 46:CM:392:C:C6    | 2.46                     | 0.49              |
| 46:CM:643:U:H2'    | 46:CM:644:U:O4'   | 2.12                     | 0.49              |
| 46:CM:1523:G:O2'   | 46:CM:1524:C:OP1  | 2.27                     | 0.49              |
| 46:CM:1544:U:H5'   | 62:DC:115:TYR:CD2 | 2.47                     | 0.49              |
| 71:DL:56:SER:HB3   | 71:DL:74:LEU:CD1  | 2.41                     | 0.49              |
| 79:DT:134:VAL:HG12 | 79:DT:142:MET:HE3 | 1.93                     | 0.49              |
| 79:DT:157:ILE:HG12 | 79:DT:158:SER:N   | 2.26                     | 0.49              |
| 79:DT:184:SER:O    | 79:DT:185:VAL:C   | 2.53                     | 0.49              |
| 1:1:371:G:N1       | 1:1:374:A:OP2     | 2.42                     | 0.49              |
| 1:1:647:A:H2'      | 1:1:648:C:C6      | 2.46                     | 0.49              |
| 1:1:779:A:H5''     | 1:1:780:A:H5''    | 1.93                     | 0.49              |
| 1:1:787:A:H2'      | 1:1:788:G:C8      | 2.47                     | 0.49              |
| 1:1:925:A:O2'      | 38:AK:49:TRP:O    | 2.30                     | 0.49              |
| 1:1:1199:A:H2'     | 1:1:1200:A:H8     | 1.76                     | 0.49              |
| 1:1:1469:G:H5''    | 20:z:23:TRP:CD1   | 2.46                     | 0.49              |
| 1:1:1802:A:H4'     | 35:AH:76:TYR:CZ   | 2.47                     | 0.49              |
| 1:1:1807:G:H2'     | 1:1:1808:G:O4'    | 2.11                     | 0.49              |
| 1:1:2329:U:H2'     | 1:1:2330:A:H8     | 1.77                     | 0.49              |
| 1:1:2420:G:H2'     | 1:1:2421:A:C8     | 2.47                     | 0.49              |
| 1:1:2516:U:O3'     | 1:1:2519:A:N6     | 2.45                     | 0.49              |
| 36:AI:8:GLU:HG2    | 27:BT:127:GLU:O   | 2.11                     | 0.49              |
| 46:B:248:C:H2'     | 46:B:249:A:C8     | 2.46                     | 0.49              |
| 46:B:261:C:H4'     | 46:B:290:U:H5'    | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:679:C:O2'    | 46:B:680:C:H4'    | 2.11                     | 0.49              |
| 46:B:933:A:H2'    | 46:B:934:C:H6     | 1.77                     | 0.49              |
| 46:B:1602:C:H5''  | 46:B:1603:G:O5'   | 2.12                     | 0.49              |
| 57:M:76:LEU:O     | 57:M:80:LEU:HB2   | 2.12                     | 0.49              |
| 59:O:38:HIS:C     | 59:O:40:GLY:N     | 2.66                     | 0.49              |
| 59:O:68:GLU:O     | 59:O:69:GLU:HG3   | 2.12                     | 0.49              |
| 65:U:132:LYS:HD3  | 65:U:136:GLN:HB2  | 1.94                     | 0.49              |
| 67:W:68:LYS:HE2   | 67:W:79:ASP:OD1   | 2.12                     | 0.49              |
| 76:f:12:ARG:HB2   | 76:f:12:ARG:HH11  | 1.77                     | 0.49              |
| 79:AR:33:LEU:HB3  | 79:AR:45:TRP:HB2  | 1.94                     | 0.49              |
| 1:AS:815:U:H2'    | 1:AS:816:A:H8     | 1.77                     | 0.49              |
| 1:AS:1376:G:OP1   | 6:AY:192:LYS:N    | 2.42                     | 0.49              |
| 1:AS:1600:A:H4'   | 1:AS:1831:A:H4'   | 1.95                     | 0.49              |
| 1:AS:3298:G:N7    | 25:BR:35:LYS:NZ   | 2.61                     | 0.49              |
| 1:AS:3300:A:H2'   | 1:AS:3301:A:C8    | 2.46                     | 0.49              |
| 13:BF:10:ARG:O    | 13:BF:133:ARG:HD3 | 2.11                     | 0.49              |
| 29:BV:95:SER:OG   | 29:BV:96:ALA:N    | 2.46                     | 0.49              |
| 36:CC:20:GLN:O    | 36:CC:24:LEU:HG   | 2.11                     | 0.49              |
| 38:CE:69:HIS:O    | 38:CE:73:ARG:HG3  | 2.11                     | 0.49              |
| 46:CM:1344:C:OP1  | 66:DG:130:ARG:HG3 | 2.11                     | 0.49              |
| 55:CV:11:ARG:O    | 58:CY:133:LYS:NZ  | 2.44                     | 0.49              |
| 56:CW:92:LYS:C    | 56:CW:94:ASP:H    | 2.20                     | 0.49              |
| 57:CX:3:ILE:HB    | 57:CX:8:ARG:HH11  | 1.77                     | 0.49              |
| 59:CZ:71:ILE:HD12 | 59:CZ:71:ILE:H    | 1.77                     | 0.49              |
| 82:12:103:ASN:HA  | 82:12:144:ASP:C   | 2.37                     | 0.49              |
| 1:1:616:C:O2'     | 1:1:619:A:N3      | 2.38                     | 0.49              |
| 1:1:2185:A:N6     | 46:B:898:G:N3     | 2.60                     | 0.49              |
| 1:1:2739:U:H2'    | 1:1:2740:U:C6     | 2.47                     | 0.49              |
| 1:1:3196:U:H2'    | 1:1:3197:G:C8     | 2.45                     | 0.49              |
| 1:1:3223:U:O2'    | 1:1:3225:G:OP1    | 2.23                     | 0.49              |
| 1:1:3313:G:H2'    | 1:1:3314:C:C6     | 2.47                     | 0.49              |
| 7:m:95:TRP:HD1    | 7:m:158:ARG:HA    | 1.77                     | 0.49              |
| 45:i:89:ASP:C     | 45:i:91:HIS:H     | 2.19                     | 0.49              |
| 46:B:255:A:H1'    | 55:K:73:SER:HB2   | 1.95                     | 0.49              |
| 46:B:982:G:C6     | 46:B:993:G:C6     | 3.00                     | 0.49              |
| 46:B:1303:G:H5''  | 64:T:67:ARG:NH1   | 2.27                     | 0.49              |
| 46:B:1456:C:H3'   | 46:B:1560:A:H62   | 1.77                     | 0.49              |
| 46:B:1635:A:H2'   | 46:B:1636:C:H6    | 1.76                     | 0.49              |
| 51:G:123:LEU:HD13 | 51:G:237:VAL:HG13 | 1.94                     | 0.49              |
| 66:V:37:VAL:HG21  | 66:V:100:ILE:HD11 | 1.94                     | 0.49              |
| 71:a:57:VAL:HB    | 71:a:60:PHE:HE2   | 1.77                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:AR:257:ILE:HB  | 79:AR:271:LEU:HB2  | 1.93                     | 0.49              |
| 1:AS:956:U:H4'    | 1:AS:959:G:N1      | 2.26                     | 0.49              |
| 1:AS:1762:G:O2'   | 1:AS:1763:C:OP1    | 2.30                     | 0.49              |
| 1:AS:1863:A:H2'   | 1:AS:1864:G:C8     | 2.48                     | 0.49              |
| 6:AY:300:VAL:HB   | 19:BL:39:ARG:CG    | 2.40                     | 0.49              |
| 17:BJ:36:VAL:HB   | 17:BJ:105:VAL:HG12 | 1.94                     | 0.49              |
| 21:BN:171:PHE:O   | 21:BN:172:TYR:HB2  | 2.12                     | 0.49              |
| 22:BO:52:MET:HA   | 22:BO:95:HIS:CE1   | 2.48                     | 0.49              |
| 25:BR:80:ARG:HD2  | 25:BR:80:ARG:N     | 2.27                     | 0.49              |
| 32:BY:95:VAL:HG12 | 32:BY:97:VAL:HG13  | 1.95                     | 0.49              |
| 46:CM:58:U:O2'    | 46:CM:449:G:N3     | 2.45                     | 0.49              |
| 46:CM:1542:A:O3'  | 62:DC:44:ARG:NH1   | 2.46                     | 0.49              |
| 46:CM:1636:C:H2'  | 46:CM:1637:U:C6    | 2.47                     | 0.49              |
| 48:CO:22:ASP:O    | 48:CO:24:PHE:N     | 2.45                     | 0.49              |
| 48:CO:82:ARG:HB3  | 48:CO:103:LEU:HD11 | 1.95                     | 0.49              |
| 56:CW:77:ILE:HG21 | 56:CW:91:MET:HB3   | 1.94                     | 0.49              |
| 72:DM:65:LEU:HD13 | 72:DM:69:LEU:HD12  | 1.93                     | 0.49              |
| 79:DT:13:LEU:HB3  | 79:DT:45:TRP:CH2   | 2.47                     | 0.49              |
| 79:DT:147:GLY:HA3 | 79:DT:178:TRP:HH2  | 1.77                     | 0.49              |
| 79:DT:182:ASP:OD1 | 79:DT:184:SER:OG   | 2.24                     | 0.49              |
| 81:P0:39:HIS:HB3  | 82:12:121:PHE:CE2  | 2.47                     | 0.49              |
| 81:P0:65:GLY:C    | 81:P0:67:LEU:H     | 2.19                     | 0.49              |
| 1:1:290:G:H1'     | 16:v:93:LYS:HD2    | 1.95                     | 0.49              |
| 1:1:430:G:H2'     | 1:1:431:A:C8       | 2.48                     | 0.49              |
| 1:1:602:A:H8      | 1:1:602:A:O5'      | 1.95                     | 0.49              |
| 1:1:907:C:OP1     | 4:j:14:SER:OG      | 2.29                     | 0.49              |
| 1:1:1921:U:O4     | 1:1:2297:U:O2'     | 2.28                     | 0.49              |
| 1:1:2429:G:H2'    | 1:1:2430:G:C8      | 2.47                     | 0.49              |
| 1:1:2437:A:H3'    | 1:1:2438:U:H5''    | 1.94                     | 0.49              |
| 1:1:3159:A:H2'    | 1:1:3160:C:C6      | 2.47                     | 0.49              |
| 2:3:70:A:H2'      | 2:3:71:U:C6        | 2.47                     | 0.49              |
| 3:4:113:U:H5''    | 40:AM:7:PHE:CB     | 2.41                     | 0.49              |
| 25:7:9:SER:HA     | 25:7:52:THR:HB     | 1.94                     | 0.49              |
| 25:7:117:LYS:O    | 25:7:118:ALA:C     | 2.54                     | 0.49              |
| 31:AD:11:ASN:HD22 | 31:AD:11:ASN:N     | 2.10                     | 0.49              |
| 46:B:151:G:O6     | 71:a:128:ARG:NH1   | 2.46                     | 0.49              |
| 46:B:233:G:H2'    | 46:B:234:G:C8      | 2.47                     | 0.49              |
| 46:B:265:U:H2'    | 46:B:266:C:C6      | 2.47                     | 0.49              |
| 46:B:479:A:H2'    | 46:B:480:U:C6      | 2.47                     | 0.49              |
| 46:B:809:G:H2'    | 46:B:810:U:H6      | 1.76                     | 0.49              |
| 46:B:1672:G:O2'   | 46:B:1673:U:H5'    | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:C:49:ASN:ND2   | 47:C:52:LYS:HG3   | 2.28                     | 0.49              |
| 50:F:24:GLU:OE1   | 76:f:23:HIS:HE1   | 1.95                     | 0.49              |
| 52:H:109:LYS:HG3  | 52:H:112:ARG:NH2  | 2.28                     | 0.49              |
| 63:S:14:THR:HB    | 63:S:71:GLY:HA2   | 1.94                     | 0.49              |
| 74:d:36:LYS:HZ1   | 74:d:43:ILE:HD13  | 1.76                     | 0.49              |
| 1:AS:243:G:H2'    | 1:AS:244:G:C8     | 2.48                     | 0.49              |
| 1:AS:612:U:H2'    | 1:AS:613:U:C6     | 2.47                     | 0.49              |
| 1:AS:671:U:H2'    | 1:AS:672:G:C8     | 2.48                     | 0.49              |
| 1:AS:1030:U:H2'   | 1:AS:1031:A:H8    | 1.77                     | 0.49              |
| 1:AS:1151:C:H2'   | 1:AS:1152:C:H6    | 1.78                     | 0.49              |
| 1:AS:2074:A:H2'   | 1:AS:2075:U:C6    | 2.47                     | 0.49              |
| 1:AS:2128:G:O2'   | 1:AS:2167:U:OP1   | 2.29                     | 0.49              |
| 1:AS:2720:A:H1'   | 7:AZ:36:LEU:HD23  | 1.94                     | 0.49              |
| 1:AS:2738:U:H2'   | 1:AS:2739:U:C6    | 2.48                     | 0.49              |
| 1:AS:2739:U:H2'   | 1:AS:2740:U:H6    | 1.77                     | 0.49              |
| 1:AS:3166:A:H2'   | 1:AS:3167:G:H5'   | 1.95                     | 0.49              |
| 3:AU:9:A:H2'      | 3:AU:10:A:H8      | 1.78                     | 0.49              |
| 46:CM:1581:G:H2'  | 46:CM:1582:U:O4'  | 2.13                     | 0.49              |
| 52:CS:72:HIS:HD2  | 63:DD:43:LEU:HD21 | 1.77                     | 0.49              |
| 1:1:583:A:H2'     | 1:1:584:C:H6      | 1.75                     | 0.49              |
| 1:1:967:G:H1      | 1:1:1106:U:H3     | 1.61                     | 0.49              |
| 1:1:1417:G:H2'    | 1:1:1418:G:H8     | 1.78                     | 0.49              |
| 1:1:1530:A:H2'    | 1:1:1531:A:C8     | 2.48                     | 0.49              |
| 1:1:1903:C:O2     | 5:k:240:ARG:NH2   | 2.45                     | 0.49              |
| 1:1:2408:A:H2'    | 1:1:2409:C:C6     | 2.47                     | 0.49              |
| 1:1:2410:A:H2     | 16:v:125:SER:HB2  | 1.78                     | 0.49              |
| 1:1:3319:U:H5''   | 1:1:3320:U:H3'    | 1.95                     | 0.49              |
| 13:s:4:LYS:HG3    | 13:s:6:GLN:H      | 1.77                     | 0.49              |
| 36:AI:100:GLU:OE1 | 36:AI:108:ARG:NE  | 2.46                     | 0.49              |
| 46:B:379:C:H5''   | 51:G:10:LYS:HD2   | 1.94                     | 0.49              |
| 46:B:944:U:C2     | 60:P:17:PRO:HG3   | 2.48                     | 0.49              |
| 46:B:1609:G:H2'   | 46:B:1610:C:H6    | 1.77                     | 0.49              |
| 46:B:1753:A:N6    | 73:c:80:HIS:HA    | 2.28                     | 0.49              |
| 62:R:60:LEU:HD21  | 62:R:94:VAL:HG12  | 1.94                     | 0.49              |
| 1:AS:445:A:H2'    | 1:AS:446:U:C6     | 2.47                     | 0.49              |
| 1:AS:564:G:H2'    | 1:AS:565:A:H8     | 1.68                     | 0.49              |
| 1:AS:785:A:H2'    | 1:AS:786:U:H6     | 1.77                     | 0.49              |
| 1:AS:925:A:H2'    | 1:AS:926:U:C6     | 2.48                     | 0.49              |
| 1:AS:1656:C:H2'   | 1:AS:1657:G:H8    | 1.78                     | 0.49              |
| 1:AS:1908:U:O2'   | 1:AS:2099:G:N7    | 2.38                     | 0.49              |
| 1:AS:2130:A:H2'   | 1:AS:2131:U:C6    | 2.47                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:2361:C:H5'    | 17:BJ:72:PHE:CE2   | 2.46                     | 0.49              |
| 1:AS:2796:G:H2'    | 1:AS:2797:C:H6     | 1.78                     | 0.49              |
| 1:AS:3019:U:O2'    | 1:AS:3020:A:H5'    | 2.11                     | 0.49              |
| 3:AU:4:C:H2'       | 3:AU:5:U:C6        | 2.47                     | 0.49              |
| 36:CC:99:GLN:OE1   | 36:CC:100:GLU:N    | 2.45                     | 0.49              |
| 42:CI:15:ARG:NE    | 46:CM:1111:G:OP1   | 2.45                     | 0.49              |
| 46:CM:50:C:N4      | 46:CM:423:A:OP2    | 2.36                     | 0.49              |
| 46:CM:874:U:H2'    | 46:CM:875:C:C6     | 2.48                     | 0.49              |
| 46:CM:1226:G:H4'   | 62:DC:77:LYS:O     | 2.13                     | 0.49              |
| 48:CO:135:LEU:HD21 | 48:CO:184:LEU:CD2  | 2.42                     | 0.49              |
| 54:CU:137:ARG:HG2  | 54:CU:139:LEU:HD22 | 1.93                     | 0.49              |
| 57:CX:3:ILE:HB     | 57:CX:8:ARG:NH1    | 2.27                     | 0.49              |
| 62:DC:125:PRO:O    | 62:DC:127:ARG:NH2  | 2.45                     | 0.49              |
| 65:DF:25:ARG:NH1   | 65:DF:25:ARG:HB3   | 2.27                     | 0.49              |
| 69:DJ:114:GLU:O    | 69:DJ:118:ARG:HG3  | 2.12                     | 0.49              |
| 79:DT:215:GLY:O    | 79:DT:233:ALA:N    | 2.34                     | 0.49              |
| 1:1:792:U:H2'      | 1:1:793:U:C6       | 2.47                     | 0.49              |
| 1:1:1456:A:H5'     | 32:AE:50:LEU:O     | 2.13                     | 0.49              |
| 1:1:2853:C:H2'     | 1:1:2854:U:H6      | 1.76                     | 0.49              |
| 1:1:2927:U:H2'     | 1:1:2928:A:O4'     | 2.13                     | 0.49              |
| 6:l:61:THR:HB      | 6:l:91:PHE:CE1     | 2.48                     | 0.49              |
| 11:q:110:ASP:HB3   | 11:q:128:ILE:HD12  | 1.95                     | 0.49              |
| 22:2:136:ARG:HB2   | 22:2:139:ARG:NH2   | 2.27                     | 0.49              |
| 25:7:113:LYS:O     | 25:7:116:LYS:HB3   | 2.13                     | 0.49              |
| 30:AC:11:ASN:O     | 30:AC:11:ASN:ND2   | 2.46                     | 0.49              |
| 32:AE:30:LYS:NZ    | 32:AE:34:GLU:OE2   | 2.45                     | 0.49              |
| 46:B:290:U:H2'     | 46:B:291:U:C6      | 2.47                     | 0.49              |
| 46:B:1604:U:H2'    | 46:B:1605:C:C6     | 2.48                     | 0.49              |
| 63:S:39:GLN:O      | 63:S:41:GLU:N      | 2.45                     | 0.49              |
| 66:V:74:GLY:HA2    | 66:V:77:ASN:HD22   | 1.77                     | 0.49              |
| 1:AS:623:A:H2'     | 1:AS:624:U:C6      | 2.48                     | 0.49              |
| 1:AS:629:A:H2      | 34:CA:91:PRO:HG2   | 1.77                     | 0.49              |
| 1:AS:1203:G:OP1    | 41:CH:43:ASN:ND2   | 2.46                     | 0.49              |
| 1:AS:1705:C:H2'    | 1:AS:1706:C:C6     | 2.47                     | 0.49              |
| 1:AS:1807:G:H2'    | 1:AS:1808:G:O4'    | 2.12                     | 0.49              |
| 1:AS:2718:A:H5'    | 7:AZ:178:ASN:OD1   | 2.12                     | 0.49              |
| 1:AS:3171:C:H5''   | 1:AS:3172:U:O5'    | 2.12                     | 0.49              |
| 1:AS:3320:U:OP2    | 55:CV:77:ARG:NH2   | 2.45                     | 0.49              |
| 9:BB:149:ARG:HD2   | 9:BB:205:LEU:HD23  | 1.93                     | 0.49              |
| 80:BE:86:HIS:ND1   | 80:BE:139:ARG:HD3  | 2.27                     | 0.49              |
| 20:BM:173:ARG:HH11 | 20:BM:173:ARG:HG3  | 1.78                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BR:99:SER:HA   | 25:BR:102:LYS:CD   | 2.43                     | 0.49              |
| 45:CL:125:ALA:HA  | 45:CL:128:GLU:OE2  | 2.12                     | 0.49              |
| 46:CM:149:G:N2    | 53:CT:13:GLN:OE1   | 2.35                     | 0.49              |
| 46:CM:222:C:C4    | 46:CM:823:G:N2     | 2.80                     | 0.49              |
| 46:CM:582:C:C4    | 46:CM:583:A:N7     | 2.80                     | 0.49              |
| 46:CM:823:G:O2'   | 46:CM:824:U:C2     | 2.59                     | 0.49              |
| 46:CM:1189:A:N3   | 76:DQ:10:HIS:NE2   | 2.60                     | 0.49              |
| 46:CM:1205:C:H2'  | 46:CM:1206:A:C8    | 2.48                     | 0.49              |
| 46:CM:1566:U:H2'  | 46:CM:1567:C:C6    | 2.48                     | 0.49              |
| 48:CO:32:ILE:HG13 | 48:CO:43:VAL:HG23  | 1.94                     | 0.49              |
| 49:CP:211:ALA:O   | 49:CP:215:ASN:ND2  | 2.40                     | 0.49              |
| 52:CS:91:GLU:O    | 52:CS:95:ASN:ND2   | 2.45                     | 0.49              |
| 62:DC:16:SER:O    | 65:DF:93:VAL:HA    | 2.12                     | 0.49              |
| 62:DC:125:PRO:HG2 | 62:DC:127:ARG:HH12 | 1.78                     | 0.49              |
| 71:DL:87:PRO:HD2  | 71:DL:90:ARG:HD2   | 1.93                     | 0.49              |
| 1:1:417:A:H2'     | 1:1:418:A:C8       | 2.48                     | 0.49              |
| 1:1:684:G:C2      | 1:1:693:C:C2       | 3.01                     | 0.49              |
| 1:1:780:A:H2      | 19:y:69:ARG:HD3    | 1.77                     | 0.49              |
| 1:1:1230:G:H5'    | 82:12:119:LYS:HB3  | 1.95                     | 0.49              |
| 1:1:2126:U:H2'    | 1:1:2127:A:N7      | 2.27                     | 0.49              |
| 1:1:2176:A:C2     | 1:1:2177:G:C8      | 3.01                     | 0.49              |
| 1:1:2638:C:OP2    | 1:1:2659:G:N2      | 2.44                     | 0.49              |
| 4:j:29:LEU:HD22   | 4:j:101:ILE:HD13   | 1.95                     | 0.49              |
| 28:AA:23:VAL:HA   | 28:AA:45:GLY:HA2   | 1.94                     | 0.49              |
| 31:AD:26:THR:HB   | 31:AD:31:SER:HB3   | 1.94                     | 0.49              |
| 34:AG:103:TYR:HA  | 34:AG:104:PRO:C    | 2.38                     | 0.49              |
| 45:i:86:LYS:NZ    | 45:i:88:PHE:O      | 2.45                     | 0.49              |
| 46:B:178:A:H2'    | 46:B:179:A:O4'     | 2.13                     | 0.49              |
| 46:B:191:U:H4'    | 46:B:192:U:H5'     | 1.94                     | 0.49              |
| 46:B:217:A:C8     | 46:B:816:U:C2      | 3.00                     | 0.49              |
| 46:B:772:A:H5''   | 46:B:773:A:O4'     | 2.12                     | 0.49              |
| 46:B:1298:A:N3    | 46:B:1300:U:H5'    | 2.27                     | 0.49              |
| 52:H:200:ASN:CB   | 52:H:208:SER:HB3   | 2.41                     | 0.49              |
| 1:AS:867:U:H5''   | 1:AS:2120:A:OP1    | 2.13                     | 0.49              |
| 1:AS:964:G:H2'    | 1:AS:965:C:H6      | 1.77                     | 0.49              |
| 1:AS:1116:A:H2'   | 1:AS:1117:U:C6     | 2.47                     | 0.49              |
| 1:AS:1789:C:OP1   | 4:AW:177:LYS:NZ    | 2.39                     | 0.49              |
| 10:BC:150:LYS:HE3 | 10:BC:202:THR:O    | 2.12                     | 0.49              |
| 14:BG:198:GLU:O   | 14:BG:201:LYS:HB2  | 2.12                     | 0.49              |
| 28:BU:84:ARG:NH1  | 35:CB:97:GLU:OE2   | 2.46                     | 0.49              |
| 46:CM:637:U:H5'   | 54:CU:97:LYS:HE3   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1050:A:C5'   | 48:CO:160:LYS:HZ1  | 2.25                     | 0.49              |
| 46:CM:1050:A:H4'   | 48:CO:205:PHE:HD1  | 1.78                     | 0.49              |
| 48:CO:105:PHE:CZ   | 48:CO:211:HIS:HB3  | 2.48                     | 0.49              |
| 50:CQ:68:HIS:CE1   | 57:CX:93:LYS:HG2   | 2.48                     | 0.49              |
| 54:CU:44:GLU:OE2   | 54:CU:52:LYS:HB3   | 2.13                     | 0.49              |
| 54:CU:69:VAL:O     | 54:CU:73:LEU:N     | 2.24                     | 0.49              |
| 56:CW:44:ARG:O     | 56:CW:48:GLN:HG3   | 2.13                     | 0.49              |
| 72:DM:64:VAL:HG13  | 72:DM:68:ARG:HH21  | 1.77                     | 0.49              |
| 78:DS:161:ARG:HH21 | 78:DS:163:CYS:C    | 2.20                     | 0.49              |
| 79:DT:71:ASP:OD1   | 79:DT:72:VAL:N     | 2.46                     | 0.49              |
| 81:P0:22:TYR:CD2   | 81:P0:88:PHE:HB3   | 2.48                     | 0.49              |
| 1:1:234:A:H2'      | 1:1:235:G:O4'      | 2.13                     | 0.49              |
| 1:1:602:A:H2'      | 1:1:603:C:C6       | 2.48                     | 0.49              |
| 1:1:657:G:H2'      | 1:1:1428:C:H42     | 1.78                     | 0.49              |
| 1:1:981:U:H2'      | 1:1:982:U:H6       | 1.76                     | 0.49              |
| 1:1:1268:C:H2'     | 1:1:1269:A:O4'     | 2.12                     | 0.49              |
| 1:1:2391:A:H2'     | 1:1:2392:G:H8      | 1.77                     | 0.49              |
| 1:1:2451:C:H3'     | 1:1:2452:G:O4'     | 2.12                     | 0.49              |
| 1:1:3164:U:H1'     | 1:1:3165:U:C4      | 2.47                     | 0.49              |
| 3:4:49:G:OP2       | 36:AI:48:ARG:NH1   | 2.46                     | 0.49              |
| 4:j:180:LEU:HD22   | 44:AQ:18:TYR:HB3   | 1.93                     | 0.49              |
| 7:m:49:TYR:CE1     | 7:m:66:SER:HB3     | 2.48                     | 0.49              |
| 10:p:255:ALA:HA    | 10:p:258:VAL:HG12  | 1.95                     | 0.49              |
| 38:AK:26:SER:HB3   | 38:AK:35:SER:OG    | 2.13                     | 0.49              |
| 46:B:1070:G:N2     | 46:B:1073:A:OP2    | 2.40                     | 0.49              |
| 46:B:1308:C:H2'    | 46:B:1309:G:C8     | 2.48                     | 0.49              |
| 46:B:1423:U:H2'    | 46:B:1424:G:C8     | 2.47                     | 0.49              |
| 46:B:1543:A:H1'    | 46:B:1547:U:OP2    | 2.13                     | 0.49              |
| 46:B:1551:U:H2'    | 46:B:1552:C:C6     | 2.47                     | 0.49              |
| 47:C:84:ARG:HE     | 64:T:82:ASP:CG     | 2.19                     | 0.49              |
| 51:G:99:PHE:HE1    | 51:G:113:ARG:HG2   | 1.78                     | 0.49              |
| 52:H:55:ASP:OD1    | 52:H:57:SER:OG     | 2.30                     | 0.49              |
| 55:K:190:LEU:HD22  | 55:K:194:GLU:HG2   | 1.93                     | 0.49              |
| 60:P:69:ASN:HB3    | 60:P:73:ARG:HD2    | 1.94                     | 0.49              |
| 79:AR:167:ILE:HG13 | 79:AR:222:LEU:HD11 | 1.95                     | 0.49              |
| 1:AS:65:A:P        | 14:BG:100:ARG:HH12 | 2.36                     | 0.49              |
| 1:AS:730:A:H8      | 1:AS:733:A:H62     | 1.59                     | 0.49              |
| 1:AS:1434:U:H4'    | 6:AY:89:ALA:CB     | 2.42                     | 0.49              |
| 1:AS:1517:G:C6     | 26:BS:116:PRO:HG2  | 2.48                     | 0.49              |
| 1:AS:2638:C:O2'    | 45:CL:40:ASP:OD2   | 2.17                     | 0.49              |
| 1:AS:2644:G:H1'    | 13:BF:97:SER:HB3   | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AT:40:C:H2'      | 2:AT:42:A:N7       | 2.27                     | 0.49              |
| 2:AT:59:U:H2'      | 2:AT:60:G:C8       | 2.48                     | 0.49              |
| 14:BG:69:VAL:CG1   | 14:BG:152:PRO:HD3  | 2.43                     | 0.49              |
| 16:BI:104:GLU:OE2  | 16:BI:161:ALA:HA   | 2.13                     | 0.49              |
| 23:BP:17:VAL:HG23  | 23:BP:64:VAL:HB    | 1.94                     | 0.49              |
| 26:BS:100:LYS:HA   | 26:BS:105:VAL:H    | 1.78                     | 0.49              |
| 37:CD:52:TYR:CE1   | 37:CD:53:GLU:HG3   | 2.48                     | 0.49              |
| 46:CM:822:G:H8     | 46:CM:822:G:O5'    | 1.95                     | 0.49              |
| 46:CM:871:U:C2     | 46:CM:872:A:C8     | 3.01                     | 0.49              |
| 46:CM:1191:U:OP2   | 46:CM:1192:C:O2'   | 2.14                     | 0.49              |
| 46:CM:1634:U:H2'   | 46:CM:1635:A:H8    | 1.78                     | 0.49              |
| 46:CM:1656:U:H2'   | 46:CM:1657:G:O4'   | 2.13                     | 0.49              |
| 48:CO:195:ARG:O    | 48:CO:199:LYS:HB2  | 2.12                     | 0.49              |
| 52:CS:114:VAL:O    | 52:CS:118:LEU:HG   | 2.13                     | 0.49              |
| 54:CU:16:LYS:O     | 54:CU:19:GLN:HB3   | 2.12                     | 0.49              |
| 59:CZ:99:GLU:OE1   | 59:CZ:100:TRP:HD1  | 1.95                     | 0.49              |
| 64:DE:66:VAL:HG13  | 64:DE:69:ILE:HG12  | 1.94                     | 0.49              |
| 68:DI:11:LEU:HD23  | 68:DI:11:LEU:H     | 1.77                     | 0.49              |
| 79:DT:151:TRP:C    | 79:DT:170:SER:HG   | 2.13                     | 0.49              |
| 79:DT:155:VAL:HG12 | 79:DT:168:SER:HB2  | 1.93                     | 0.49              |
| 79:DT:261:LYS:HE2  | 79:DT:266:SER:HB2  | 1.95                     | 0.49              |
| 1:1:37:U:H2'       | 1:1:38:A:O4'       | 2.12                     | 0.49              |
| 1:1:273:A:H2'      | 1:1:274:G:C8       | 2.47                     | 0.49              |
| 1:1:1252:G:O2'     | 82:12:120:SER:OG   | 2.18                     | 0.49              |
| 1:1:1593:C:H5'     | 1:1:1692:A:H1'     | 1.95                     | 0.49              |
| 1:1:2978:A:H2'     | 1:1:2979:U:O4'     | 2.13                     | 0.49              |
| 3:4:8:C:H2'        | 3:4:9:A:C8         | 2.48                     | 0.49              |
| 5:k:117:ARG:HD2    | 5:k:176:ALA:O      | 2.13                     | 0.49              |
| 33:AF:112:LYS:HE2  | 33:AF:116:LEU:HD11 | 1.95                     | 0.49              |
| 46:B:347:U:OP1     | 58:N:104:HIS:NE2   | 2.43                     | 0.49              |
| 46:B:1396:A:O2'    | 46:B:1397:A:OP1    | 2.28                     | 0.49              |
| 46:B:1539:U:O2'    | 46:B:1584:A:N3     | 2.40                     | 0.49              |
| 62:R:52:LYS:HB2    | 62:R:53:PRO:HD3    | 1.95                     | 0.49              |
| 1:AS:212:A:OP1     | 27:BT:2:ALA:N      | 2.46                     | 0.49              |
| 1:AS:941:C:H2'     | 1:AS:942:U:H6      | 1.77                     | 0.49              |
| 1:AS:1045:C:H2'    | 1:AS:1046:U:C6     | 2.48                     | 0.49              |
| 1:AS:1157:G:O2'    | 33:BZ:55:ASN:OD1   | 2.26                     | 0.49              |
| 1:AS:2339:A:H2'    | 1:AS:2340:C:H6     | 1.77                     | 0.49              |
| 1:AS:2354:G:H2'    | 1:AS:2355:G:C8     | 2.48                     | 0.49              |
| 1:AS:2419:A:H2'    | 1:AS:2420:G:H8     | 1.78                     | 0.49              |
| 7:AZ:6:GLU:OE1     | 7:AZ:7:PHE:N       | 2.46                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:BC:137:LEU:CD2 | 10:BC:163:LEU:HB3  | 2.42                     | 0.49              |
| 35:CB:98:GLN:O    | 35:CB:102:LYS:HG2  | 2.13                     | 0.49              |
| 46:CM:146:A:H61   | 53:CT:133:LEU:HD12 | 1.78                     | 0.49              |
| 46:CM:483:A:H2'   | 46:CM:484:G:H8     | 1.75                     | 0.49              |
| 46:CM:740:A:H2'   | 46:CM:741:A:H8     | 1.78                     | 0.49              |
| 46:CM:874:U:H2'   | 46:CM:875:C:H6     | 1.78                     | 0.49              |
| 46:CM:1039:U:O2'  | 48:CO:147:PRO:HG2  | 2.13                     | 0.49              |
| 46:CM:1337:C:H2'  | 46:CM:1338:U:O4'   | 2.13                     | 0.49              |
| 47:CN:63:ILE:HG12 | 68:DI:36:ILE:HG22  | 1.95                     | 0.49              |
| 48:CO:34:ALA:HB3  | 48:CO:41:ARG:HA    | 1.95                     | 0.49              |
| 48:CO:81:TYR:OH   | 48:CO:82:ARG:NH2   | 2.42                     | 0.49              |
| 48:CO:219:LYS:HZ2 | 48:CO:220:GLN:C    | 2.16                     | 0.49              |
| 52:CS:135:ASP:HB2 | 52:CS:202:ALA:HB1  | 1.94                     | 0.49              |
| 52:CS:145:ASP:OD2 | 75:DP:45:LYS:HE2   | 2.13                     | 0.49              |
| 57:CX:61:TRP:CZ2  | 76:DQ:23:HIS:CE1   | 3.01                     | 0.49              |
| 59:CZ:67:THR:HG23 | 59:CZ:68:GLU:OE1   | 2.13                     | 0.49              |
| 67:DH:27:SER:OG   | 67:DH:111:VAL:HA   | 2.13                     | 0.49              |
| 77:DR:4:VAL:HG23  | 77:DR:5:HIS:ND1    | 2.28                     | 0.49              |
| 79:DT:91:ARG:HD2  | 79:DT:93:TRP:CH2   | 2.48                     | 0.49              |
| 79:DT:284:PRO:CG  | 79:DT:304:ASP:HB3  | 2.42                     | 0.49              |
| 1:1:40:G:N2       | 1:1:2775:A:H62     | 2.11                     | 0.49              |
| 1:1:951:U:H2'     | 1:1:952:U:C6       | 2.48                     | 0.49              |
| 1:1:1176:A:C4     | 1:1:1178:G:C8      | 3.01                     | 0.49              |
| 1:1:1357:U:H2'    | 1:1:1358:C:C6      | 2.48                     | 0.49              |
| 1:1:2472:A:H3'    | 1:1:2473:C:H5''    | 1.94                     | 0.49              |
| 1:1:2925:U:H2'    | 1:1:2926:U:H2'     | 1.95                     | 0.49              |
| 6:l:220:LEU:HD22  | 6:l:226:VAL:HG11   | 1.94                     | 0.49              |
| 15:u:21:VAL:HG22  | 15:u:55:ILE:HG22   | 1.95                     | 0.49              |
| 21:0:12:ARG:HB3   | 21:0:24:LEU:HD23   | 1.93                     | 0.49              |
| 46:B:875:C:H2'    | 46:B:876:A:C8      | 2.48                     | 0.49              |
| 46:B:1138:G:OP1   | 73:c:85:ARG:NH1    | 2.44                     | 0.49              |
| 54:J:81:PHE:HB3   | 54:J:84:ARG:HG3    | 1.95                     | 0.49              |
| 60:P:26:PHE:CE1   | 60:P:28:LEU:HB2    | 2.48                     | 0.49              |
| 61:Q:73:ALA:HB2   | 61:Q:106:ARG:HB2   | 1.95                     | 0.49              |
| 61:Q:107:ILE:HG13 | 73:c:53:LEU:HD23   | 1.95                     | 0.49              |
| 63:S:27:LEU:HD11  | 63:S:29:LYS:HZ3    | 1.77                     | 0.49              |
| 65:U:96:LYS:HB2   | 65:U:98:TYR:HE1    | 1.77                     | 0.49              |
| 1:AS:379:C:H2'    | 1:AS:380:U:H6      | 1.78                     | 0.49              |
| 1:AS:994:A:H4'    | 2:AT:103:A:C2      | 2.48                     | 0.49              |
| 1:AS:1767:G:H2'   | 1:AS:1768:U:O4'    | 2.12                     | 0.49              |
| 6:AY:6:GLN:HB2    | 6:AY:20:GLN:OE1    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:BG:58:VAL:HG12 | 14:BG:101:ARG:NH1  | 2.28                     | 0.49              |
| 15:BH:39:LEU:HD22 | 21:BN:72:VAL:HG23  | 1.94                     | 0.49              |
| 15:BH:57:LEU:HG   | 21:BN:172:TYR:OH   | 2.13                     | 0.49              |
| 17:BJ:151:GLU:O   | 17:BJ:155:GLU:HG2  | 2.12                     | 0.49              |
| 23:BP:20:ALA:N    | 23:BP:62:ASN:OD1   | 2.46                     | 0.49              |
| 23:BP:90:ASN:O    | 23:BP:92:ILE:HG23  | 2.13                     | 0.49              |
| 28:BU:15:ARG:HE   | 28:BU:79:HIS:CD2   | 2.30                     | 0.49              |
| 28:BU:98:SER:O    | 28:BU:102:GLU:OE1  | 2.31                     | 0.49              |
| 36:CC:50:ASN:O    | 36:CC:54:VAL:HG23  | 2.12                     | 0.49              |
| 46:CM:151:G:C6    | 46:CM:160:A:C6     | 3.01                     | 0.49              |
| 46:CM:1128:A:O2'  | 46:CM:1285:A:N1    | 2.43                     | 0.49              |
| 48:CO:216:LYS:HD2 | 48:CO:218:LEU:HD22 | 1.95                     | 0.49              |
| 51:CR:21:ASP:OD2  | 51:CR:24:SER:OG    | 2.31                     | 0.49              |
| 54:CU:4:LYS:HG3   | 54:CU:21:PHE:HD2   | 1.78                     | 0.49              |
| 62:DC:15:PHE:CE2  | 62:DC:17:PHE:HB2   | 2.48                     | 0.49              |
| 62:DC:83:MET:HB3  | 62:DC:116:LEU:HD22 | 1.95                     | 0.49              |
| 79:DT:135:TRP:CE2 | 79:DT:141:CYS:HB2  | 2.48                     | 0.49              |
| 1:1:294:U:P       | 16:v:15:GLN:HE22   | 2.36                     | 0.48              |
| 1:1:1383:G:O6     | 6:l:187:LYS:HD3    | 2.12                     | 0.48              |
| 1:1:1468:U:H5'    | 20:z:4:LEU:HB2     | 1.95                     | 0.48              |
| 1:1:2136:A:O2'    | 4:j:118:GLU:OE1    | 2.26                     | 0.48              |
| 1:1:3244:A:O2'    | 1:1:3245:A:H5'     | 2.13                     | 0.48              |
| 2:3:85:G:H1'      | 9:o:218:GLN:OE1    | 2.12                     | 0.48              |
| 5:k:160:VAL:HB    | 5:k:183:ILE:HD11   | 1.96                     | 0.48              |
| 8:n:71:ASN:ND2    | 8:n:159:LEU:O      | 2.45                     | 0.48              |
| 11:q:173:ARG:HD3  | 41:AN:49:LYS:O     | 2.12                     | 0.48              |
| 21:0:155:ARG:NH2  | 21:0:171:PHE:O     | 2.46                     | 0.48              |
| 33:AF:33:TRP:CH2  | 33:AF:53:GLN:HG2   | 2.48                     | 0.48              |
| 46:B:940:A:H4'    | 46:B:1058:G:O2'    | 2.13                     | 0.48              |
| 49:E:139:TRP:CE2  | 69:Y:97:ARG:HD2    | 2.47                     | 0.48              |
| 50:F:209:ILE:HD12 | 64:T:16:LEU:HD21   | 1.94                     | 0.48              |
| 52:H:57:SER:HA    | 75:e:53:ILE:HB     | 1.95                     | 0.48              |
| 64:T:25:THR:HG23  | 64:T:27:ASP:H      | 1.78                     | 0.48              |
| 67:W:81:TYR:HB3   | 76:f:52:PHE:HB3    | 1.94                     | 0.48              |
| 79:AR:263:GLN:O   | 79:AR:264:GLU:HG2  | 2.13                     | 0.48              |
| 1:AS:745:C:H5''   | 30:BW:32:LEU:HD12  | 1.93                     | 0.48              |
| 1:AS:783:G:H2'    | 1:AS:784:C:H6      | 1.77                     | 0.48              |
| 1:AS:1518:U:H3'   | 26:BS:113:LEU:HD11 | 1.94                     | 0.48              |
| 2:AT:91:G:H2'     | 2:AT:92:A:C8       | 2.48                     | 0.48              |
| 3:AU:155:G:C5     | 3:AU:156:U:C4      | 3.01                     | 0.48              |
| 7:AZ:98:ALA:HB1   | 7:AZ:162:VAL:HG23  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:BG:127:ASP:HA  | 36:CC:114:ARG:NH2  | 2.27                     | 0.48              |
| 46:CM:700:G:O2'   | 46:CM:701:G:O5'    | 2.31                     | 0.48              |
| 46:CM:1127:A:H2'  | 46:CM:1128:A:C8    | 2.48                     | 0.48              |
| 46:CM:1315:G:H2'  | 46:CM:1316:A:H8    | 1.78                     | 0.48              |
| 46:CM:1481:C:H2'  | 46:CM:1482:C:C6    | 2.48                     | 0.48              |
| 46:CM:1512:A:H5'  | 66:DG:93:HIS:HB2   | 1.95                     | 0.48              |
| 52:CS:143:ARG:NH2 | 52:CS:214:LYS:HD3  | 2.28                     | 0.48              |
| 62:DC:18:LYS:N    | 65:DF:92:GLN:O     | 2.46                     | 0.48              |
| 1:1:266:C:N4      | 37:AJ:29:LYS:HA    | 2.27                     | 0.48              |
| 1:1:706:G:N2      | 1:1:709:A:OP2      | 2.41                     | 0.48              |
| 1:1:1151:C:H2'    | 1:1:1152:C:H6      | 1.77                     | 0.48              |
| 1:1:1166:A:OP1    | 9:o:215:ARG:HA     | 2.12                     | 0.48              |
| 1:1:1501:C:P      | 18:x:23:ARG:HH12   | 2.35                     | 0.48              |
| 1:1:1834:C:H4'    | 1:1:1835:A:O4'     | 2.13                     | 0.48              |
| 1:1:2345:A:H2'    | 1:1:2346:A:H8      | 1.78                     | 0.48              |
| 1:1:2919:G:N3     | 5:k:250:ALA:HB1    | 2.28                     | 0.48              |
| 1:1:2937:U:O2     | 4:j:221:LYS:NZ     | 2.35                     | 0.48              |
| 1:1:3193:C:H4'    | 1:1:3194:G:O5'     | 2.13                     | 0.48              |
| 1:1:3285:A:H2'    | 1:1:3286:C:H6      | 1.78                     | 0.48              |
| 5:k:218:ILE:HB    | 5:k:337:THR:HB     | 1.94                     | 0.48              |
| 6:l:140:GLY:O     | 6:l:142:ARG:NH1    | 2.46                     | 0.48              |
| 46:B:139:U:P      | 53:I:149:LYS:HZ1   | 2.32                     | 0.48              |
| 46:B:817:U:HO2'   | 46:B:818:U:H6      | 1.60                     | 0.48              |
| 46:B:1181:A:H4'   | 46:B:1182:C:H5''   | 1.94                     | 0.48              |
| 46:B:1366:U:O2'   | 46:B:1503:A:N1     | 2.43                     | 0.48              |
| 51:G:123:LEU:HD23 | 51:G:159:THR:HG21  | 1.96                     | 0.48              |
| 76:f:39:CYS:HB2   | 76:f:42:CYS:HB2    | 1.95                     | 0.48              |
| 1:AS:180:U:H4'    | 38:CE:75:LYS:HG2   | 1.95                     | 0.48              |
| 1:AS:411:U:H2'    | 1:AS:412:G:C8      | 2.47                     | 0.48              |
| 1:AS:755:U:H2'    | 1:AS:756:G:O4'     | 2.13                     | 0.48              |
| 1:AS:908:G:N7     | 4:AW:9:ARG:NH2     | 2.62                     | 0.48              |
| 1:AS:1344:U:OP2   | 19:BL:38:ARG:NH2   | 2.35                     | 0.48              |
| 3:AU:122:U:H3     | 3:AU:131:G:H1      | 1.61                     | 0.48              |
| 23:BP:12:VAL:HA   | 23:BP:69:SER:HA    | 1.95                     | 0.48              |
| 39:CF:46:ARG:HH11 | 39:CF:47:GLY:H     | 1.60                     | 0.48              |
| 46:CM:182:C:H2'   | 46:CM:183:C:C6     | 2.48                     | 0.48              |
| 46:CM:577:A:H2'   | 50:CQ:144:ARG:HH22 | 1.77                     | 0.48              |
| 46:CM:653:G:O2'   | 46:CM:655:U:O4     | 2.31                     | 0.48              |
| 46:CM:885:A:H2'   | 46:CM:886:G:H8     | 1.78                     | 0.48              |
| 46:CM:932:U:H2'   | 46:CM:933:A:C8     | 2.47                     | 0.48              |
| 46:CM:1168:A:C2   | 62:DC:100:LYS:HB2  | 2.49                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 86:CM:1822:GET:H511 | 86:CM:1822:GET:H322 | 1.77                     | 0.48              |
| 47:CN:15:LYS:HZ1    | 64:DE:93:LEU:HD13   | 1.78                     | 0.48              |
| 54:CU:4:LYS:HD2     | 54:CU:37:LEU:O      | 2.13                     | 0.48              |
| 62:DC:111:MET:HE2   | 62:DC:119:PHE:CD1   | 2.48                     | 0.48              |
| 66:DG:15:ILE:HG23   | 66:DG:59:ALA:HB3    | 1.94                     | 0.48              |
| 79:DT:93:TRP:CD1    | 79:DT:93:TRP:H      | 2.30                     | 0.48              |
| 79:DT:273:PRO:HA    | 79:DT:310:TRP:HZ2   | 1.78                     | 0.48              |
| 1:1:498:C:H5''      | 8:n:25:ARG:NH2      | 2.28                     | 0.48              |
| 1:1:2380:A:H5''     | 6:l:68:THR:OG1      | 2.13                     | 0.48              |
| 1:1:3238:A:H1'      | 8:n:82:TYR:CE2      | 2.47                     | 0.48              |
| 7:m:50:ARG:NH2      | 7:m:72:ASP:OD2      | 2.47                     | 0.48              |
| 14:t:83:VAL:HG23    | 14:t:85:ILE:HG13    | 1.96                     | 0.48              |
| 30:AC:57:ALA:O      | 30:AC:58:ARG:C      | 2.55                     | 0.48              |
| 45:i:118:GLU:HB2    | 50:F:125:ARG:HG3    | 1.95                     | 0.48              |
| 47:C:10:THR:OG1     | 47:C:12:GLU:OE1     | 2.28                     | 0.48              |
| 53:I:48:TYR:CD2     | 53:I:117:GLY:HA3    | 2.48                     | 0.48              |
| 79:AR:174:THR:HG22  | 79:AR:190:ILE:HG22  | 1.95                     | 0.48              |
| 1:AS:385:A:H2'      | 1:AS:386:A:C8       | 2.48                     | 0.48              |
| 1:AS:436:A:H2'      | 1:AS:437:G:C8       | 2.49                     | 0.48              |
| 1:AS:437:G:O2'      | 1:AS:438:A:H5''     | 2.13                     | 0.48              |
| 1:AS:1923:G:N7      | 44:CK:16:VAL:HG13   | 2.29                     | 0.48              |
| 1:AS:2740:U:H2'     | 1:AS:2741:A:C8      | 2.48                     | 0.48              |
| 1:AS:3084:G:O6      | 1:AS:3092:C:H5''    | 2.12                     | 0.48              |
| 3:AU:6:U:H2'        | 3:AU:7:U:H6         | 1.78                     | 0.48              |
| 3:AU:139:U:H2'      | 3:AU:140:G:C8       | 2.48                     | 0.48              |
| 14:BG:56:PRO:HG3    | 14:BG:74:GLY:C      | 2.38                     | 0.48              |
| 36:CC:54:VAL:O      | 36:CC:58:ILE:HG13   | 2.13                     | 0.48              |
| 36:CC:86:ARG:O      | 36:CC:90:ARG:HD3    | 2.13                     | 0.48              |
| 46:CM:69:G:H2'      | 46:CM:70:C:C6       | 2.48                     | 0.48              |
| 46:CM:73:U:H4'      | 46:CM:74:U:OP1      | 2.13                     | 0.48              |
| 46:CM:167:A:OP2     | 46:CM:167:A:H8      | 1.96                     | 0.48              |
| 46:CM:384:G:H2'     | 46:CM:385:A:C8      | 2.48                     | 0.48              |
| 46:CM:518:A:O2'     | 46:CM:519:A:OP1     | 2.27                     | 0.48              |
| 46:CM:672:U:H1'     | 46:CM:673:A:C5      | 2.48                     | 0.48              |
| 46:CM:694:C:C3'     | 46:CM:695:C:H5''    | 2.28                     | 0.48              |
| 46:CM:736:G:H2'     | 46:CM:737:A:H8      | 1.78                     | 0.48              |
| 46:CM:1376:U:C6     | 64:DE:3:ARG:HG3     | 2.47                     | 0.48              |
| 57:CX:8:ARG:HG2     | 57:CX:12:HIS:CE1    | 2.48                     | 0.48              |
| 79:DT:234:LYS:HD2   | 79:DT:255:SER:OG    | 2.13                     | 0.48              |
| 81:P0:16:ARG:HA     | 81:P0:19:LEU:HB2    | 1.94                     | 0.48              |
| 1:1:15:A:OP1        | 26:8:42:ARG:HG2     | 2.13                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1:79:G:H2'       | 1:1:80:C:H6       | 1.79                     | 0.48              |
| 1:1:222:U:OP1      | 1:1:224:C:N4      | 2.35                     | 0.48              |
| 1:1:2171:U:O4      | 1:1:2221:A:N6     | 2.46                     | 0.48              |
| 1:1:3309:A:H2      | 1:1:3326:G:H21    | 1.61                     | 0.48              |
| 5:k:292:ALA:HB1    | 5:k:295:ALA:HB3   | 1.96                     | 0.48              |
| 17:w:160:LYS:O     | 17:w:164:GLN:HG3  | 2.13                     | 0.48              |
| 25:7:102:LYS:HG3   | 25:7:106:ASP:OD1  | 2.13                     | 0.48              |
| 36:AI:11:THR:O     | 27:BT:125:LYS:HE2 | 2.14                     | 0.48              |
| 46:B:16:G:H2'      | 46:B:17:C:C6      | 2.47                     | 0.48              |
| 46:B:332:G:OP2     | 55:K:54:LYS:NZ    | 2.42                     | 0.48              |
| 46:B:810:U:H2'     | 46:B:811:U:O4'    | 2.13                     | 0.48              |
| 46:B:953:U:H2'     | 46:B:954:C:O4'    | 2.12                     | 0.48              |
| 46:B:1241:A:H5'    | 46:B:1242:U:C6    | 2.48                     | 0.48              |
| 46:B:1302:C:H2'    | 46:B:1303:G:O4'   | 2.13                     | 0.48              |
| 53:I:56:ASN:ND2    | 53:I:60:GLY:O     | 2.46                     | 0.48              |
| 1:AS:73:G:C8       | 14:BG:104:LYS:NZ  | 2.81                     | 0.48              |
| 1:AS:988:A:O2'     | 1:AS:989:G:H5'    | 2.13                     | 0.48              |
| 1:AS:1291:G:H4'    | 21:BN:115:ARG:HG2 | 1.94                     | 0.48              |
| 1:AS:1561:U:H6     | 1:AS:1561:U:H5''  | 1.78                     | 0.48              |
| 1:AS:1651:G:OP1    | 35:CB:40:SER:OG   | 2.28                     | 0.48              |
| 1:AS:2999:A:H2'    | 1:AS:3000:G:O4'   | 2.13                     | 0.48              |
| 1:AS:3146:G:C6     | 1:AS:3178:A:C2    | 3.02                     | 0.48              |
| 8:BA:170:ARG:HB3   | 8:BA:172:HIS:CE1  | 2.49                     | 0.48              |
| 46:CM:30:G:H4'     | 70:DK:131:SER:HB2 | 1.96                     | 0.48              |
| 46:CM:452:A:H4'    | 51:CR:62:LYS:HE3  | 1.96                     | 0.48              |
| 46:CM:737:A:OP1    | 51:CR:187:ARG:NE  | 2.44                     | 0.48              |
| 46:CM:1235:U:O2'   | 78:DS:177:MET:HE3 | 2.12                     | 0.48              |
| 46:CM:1285:A:H5''  | 49:CP:81:VAL:HG11 | 1.96                     | 0.48              |
| 53:CT:30:LYS:NZ    | 53:CT:36:VAL:HG12 | 2.29                     | 0.48              |
| 54:CU:129:THR:HG22 | 54:CU:155:SER:HA  | 1.94                     | 0.48              |
| 60:DA:38:ILE:HD11  | 60:DA:78:ASN:ND2  | 2.29                     | 0.48              |
| 75:DP:43:ASN:ND2   | 75:DP:66:LEU:HD13 | 2.27                     | 0.48              |
| 78:DS:162:GLU:HG3  | 78:DS:163:CYS:H   | 1.78                     | 0.48              |
| 1:1:245:G:H3'      | 1:1:246:U:C6      | 2.47                     | 0.48              |
| 1:1:307:A:H2'      | 1:1:308:A:H8      | 1.73                     | 0.48              |
| 1:1:436:A:H2'      | 1:1:437:G:C8      | 2.48                     | 0.48              |
| 1:1:788:G:H2'      | 1:1:789:C:H6      | 1.79                     | 0.48              |
| 1:1:798:C:H2'      | 1:1:799:C:C6      | 2.48                     | 0.48              |
| 1:1:1308:C:O2'     | 17:w:84:ALA:O     | 2.31                     | 0.48              |
| 1:1:2236:U:C2      | 1:1:2237:A:C8     | 3.01                     | 0.48              |
| 1:1:3264:C:H2'     | 1:1:3265:U:C6     | 2.49                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:1:3281:A:C6      | 5:k:124:LYS:HG2   | 2.48                     | 0.48              |
| 15:u:20:LEU:HD23   | 15:u:21:VAL:N     | 2.29                     | 0.48              |
| 15:u:62:LEU:HD21   | 15:u:77:LYS:HB3   | 1.95                     | 0.48              |
| 36:AI:118:ILE:HG22 | 36:AI:119:LYS:N   | 2.28                     | 0.48              |
| 45:i:93:ARG:HG2    | 46:B:1259:C:C5    | 2.49                     | 0.48              |
| 46:B:103:A:O3'     | 46:B:306:C:N4     | 2.46                     | 0.48              |
| 47:C:197:VAL:HG13  | 47:C:201:LEU:HD23 | 1.94                     | 0.48              |
| 54:J:72:ARG:HG2    | 54:J:75:ARG:HH21  | 1.77                     | 0.48              |
| 56:L:34:TYR:HA     | 56:L:122:ILE:CD1  | 2.41                     | 0.48              |
| 58:N:99:ARG:HG2    | 70:Z:9:LEU:HA     | 1.94                     | 0.48              |
| 67:W:16:GLN:OE1    | 67:W:19:HIS:NE2   | 2.35                     | 0.48              |
| 68:X:79:LEU:HD13   | 68:X:82:VAL:HG11  | 1.96                     | 0.48              |
| 78:h:167:THR:HG23  | 78:h:168:CYS:SG   | 2.54                     | 0.48              |
| 1:AS:496:A:H4'     | 8:BA:27:GLN:HG3   | 1.95                     | 0.48              |
| 1:AS:538:G:O6      | 1:AS:547:U:O4     | 2.31                     | 0.48              |
| 1:AS:539:G:N1      | 1:AS:547:U:C2     | 2.81                     | 0.48              |
| 1:AS:785:A:H2'     | 1:AS:786:U:C6     | 2.49                     | 0.48              |
| 1:AS:1206:U:H5''   | 11:BD:62:ARG:HD3  | 1.95                     | 0.48              |
| 1:AS:1303:G:H4'    | 1:AS:1304:A:O5'   | 2.13                     | 0.48              |
| 1:AS:3066:A:H2'    | 1:AS:3067:U:C6    | 2.48                     | 0.48              |
| 2:AT:26:C:H2'      | 2:AT:27:A:O4'     | 2.13                     | 0.48              |
| 3:AU:8:C:H2'       | 3:AU:9:A:H8       | 1.77                     | 0.48              |
| 9:BB:108:GLN:HB2   | 19:BL:3:ARG:HD3   | 1.95                     | 0.48              |
| 15:BH:20:LEU:HD23  | 15:BH:21:VAL:N    | 2.28                     | 0.48              |
| 23:BP:19:VAL:HB    | 23:BP:62:ASN:CB   | 2.32                     | 0.48              |
| 37:CD:4:SER:N      | 37:CD:11:ASN:O    | 2.46                     | 0.48              |
| 46:CM:273:C:H2'    | 46:CM:274:C:O4'   | 2.14                     | 0.48              |
| 46:CM:445:U:H2'    | 46:CM:446:C:O4'   | 2.13                     | 0.48              |
| 46:CM:821:U:H2'    | 46:CM:822:G:H8    | 1.77                     | 0.48              |
| 46:CM:879:U:H1'    | 61:DB:31:LYS:NZ   | 2.29                     | 0.48              |
| 46:CM:1542:A:OP1   | 62:DC:47:ARG:NE   | 2.47                     | 0.48              |
| 48:CO:107:SER:O    | 48:CO:111:ARG:HG2 | 2.12                     | 0.48              |
| 50:CQ:124:LEU:HD21 | 50:CQ:153:TYR:O   | 2.13                     | 0.48              |
| 54:CU:118:HIS:ND1  | 54:CU:175:LYS:NZ  | 2.61                     | 0.48              |
| 55:CV:158:ILE:HA   | 58:CY:24:LYS:HD3  | 1.94                     | 0.48              |
| 79:DT:135:TRP:HA   | 79:DT:140:GLU:O   | 2.11                     | 0.48              |
| 79:DT:157:ILE:HG12 | 79:DT:158:SER:H   | 1.77                     | 0.48              |
| 79:DT:201:LEU:H    | 79:DT:201:LEU:CD2 | 2.08                     | 0.48              |
| 1:1:314:U:H2'      | 1:1:315:C:C6      | 2.49                     | 0.48              |
| 1:1:1139:A:H5'     | 1:1:1364:U:H1'    | 1.96                     | 0.48              |
| 1:1:1466:U:H2'     | 1:1:1467:U:C6     | 2.49                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:1892:A:H61     | 1:1:2317:C:N4      | 2.09                     | 0.48              |
| 1:1:2504:C:H2'     | 1:1:2505:G:H8      | 1.78                     | 0.48              |
| 2:3:4:U:H2'        | 2:3:5:G:C8         | 2.48                     | 0.48              |
| 3:4:70:G:P         | 27:9:121:ARG:HH22  | 2.37                     | 0.48              |
| 3:4:119:C:H2'      | 3:4:120:U:C6       | 2.48                     | 0.48              |
| 4:j:30:ARG:HG2     | 4:j:74:GLU:HG3     | 1.95                     | 0.48              |
| 6:l:17:GLY:C       | 6:l:19:SER:H       | 2.21                     | 0.48              |
| 7:m:94:ASN:HB2     | 7:m:97:ALA:H       | 1.79                     | 0.48              |
| 18:x:29:THR:HG22   | 18:x:119:VAL:HG21  | 1.95                     | 0.48              |
| 20:z:77:GLY:O      | 20:z:81:ARG:HG3    | 2.14                     | 0.48              |
| 20:z:170:ARG:HD3   | 20:z:170:ARG:N     | 2.29                     | 0.48              |
| 36:AI:59:ASN:O     | 36:AI:63:ARG:HG3   | 2.13                     | 0.48              |
| 37:AJ:49:LEU:HD22  | 37:AJ:53:GLU:HB3   | 1.95                     | 0.48              |
| 46:B:194:G:C2      | 46:B:195:A:H1'     | 2.48                     | 0.48              |
| 46:B:962:A:H2'     | 46:B:963:A:O4'     | 2.13                     | 0.48              |
| 46:B:1140:G:H2'    | 46:B:1141:C:C6     | 2.48                     | 0.48              |
| 46:B:1537:A:C6     | 46:B:1549:G:C6     | 3.01                     | 0.48              |
| 46:B:1654:A:H2'    | 46:B:1655:G:C8     | 2.48                     | 0.48              |
| 70:Z:73:ARG:NH1    | 70:Z:84:THR:OG1    | 2.41                     | 0.48              |
| 1:AS:243:G:O3'     | 14:BG:132:ALA:HB2  | 2.13                     | 0.48              |
| 1:AS:398:A:H5'     | 18:BK:3:ARG:HD3    | 1.94                     | 0.48              |
| 1:AS:406:G:H1'     | 3:AU:16:G:N2       | 2.28                     | 0.48              |
| 1:AS:602:A:H2'     | 1:AS:603:C:C6      | 2.48                     | 0.48              |
| 1:AS:813:A:H8      | 38:CE:15:SER:HG    | 1.61                     | 0.48              |
| 1:AS:2234:A:H62    | 46:CM:1743:A:H2'   | 1.77                     | 0.48              |
| 1:AS:3256:G:H2'    | 1:AS:3257:A:H8     | 1.79                     | 0.48              |
| 3:AU:45:C:OP1      | 40:CG:12:LYS:HD2   | 2.13                     | 0.48              |
| 14:BG:55:ARG:NH1   | 14:BG:73:ARG:O     | 2.39                     | 0.48              |
| 14:BG:124:VAL:HG11 | 14:BG:138:PHE:CE2  | 2.48                     | 0.48              |
| 36:CC:36:LEU:HB2   | 36:CC:37:GLN:NE2   | 2.29                     | 0.48              |
| 46:CM:1:U:H1'      | 49:CP:174:VAL:HG13 | 1.94                     | 0.48              |
| 46:CM:182:C:H2'    | 46:CM:183:C:H6     | 1.78                     | 0.48              |
| 46:CM:830:G:C6     | 46:CM:831:G:C2     | 3.01                     | 0.48              |
| 46:CM:1341:U:H2'   | 46:CM:1342:A:C8    | 2.48                     | 0.48              |
| 48:CO:22:ASP:C     | 48:CO:24:PHE:N     | 2.71                     | 0.48              |
| 54:CU:94:ILE:HG21  | 54:CU:114:LEU:CD1  | 2.44                     | 0.48              |
| 54:CU:142:GLY:O    | 54:CU:143:ASN:C    | 2.57                     | 0.48              |
| 78:DS:175:ALA:O    | 78:DS:176:ASN:C    | 2.56                     | 0.48              |
| 1:1:3079:U:H2'     | 1:1:3080:G:C8      | 2.47                     | 0.48              |
| 2:3:77:G:N2        | 2:3:102:A:OP2      | 2.26                     | 0.48              |
| 10:p:123:ALA:HA    | 10:p:126:VAL:HG22  | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:q:114:ILE:HB    | 11:q:124:ARG:HB2   | 1.95                     | 0.48              |
| 13:s:19:LEU:O      | 13:s:68:HIS:HA     | 2.13                     | 0.48              |
| 25:7:97:LYS:C      | 25:7:99:SER:H      | 2.20                     | 0.48              |
| 25:7:107:SER:OG    | 25:7:108:LYS:N     | 2.46                     | 0.48              |
| 46:B:184:C:H2'     | 46:B:185:G:O4'     | 2.14                     | 0.48              |
| 46:B:296:C:H5''    | 51:G:38:LEU:HB2    | 1.95                     | 0.48              |
| 46:B:876:A:H2'     | 46:B:877:G:C8      | 2.42                     | 0.48              |
| 46:B:1131:G:H2'    | 46:B:1132:A:H8     | 1.73                     | 0.48              |
| 51:G:100:ARG:HB2   | 51:G:114:ILE:HD13  | 1.94                     | 0.48              |
| 71:a:63:GLN:CD     | 71:a:68:LYS:HD3    | 2.38                     | 0.48              |
| 1:AS:117:U:O2      | 1:AS:120:A:H5''    | 2.13                     | 0.48              |
| 1:AS:1738:U:H2'    | 1:AS:1739:G:H8     | 1.78                     | 0.48              |
| 1:AS:2649:G:H2'    | 1:AS:2649:G:N3     | 2.29                     | 0.48              |
| 1:AS:2874:A:H2'    | 1:AS:2875:A:O4'    | 2.13                     | 0.48              |
| 6:AY:251:TRP:CZ3   | 6:AY:259:LEU:HD11  | 2.49                     | 0.48              |
| 80:BE:140:THR:HG21 | 80:BE:148:VAL:HG21 | 1.95                     | 0.48              |
| 18:BK:60:PHE:HB3   | 18:BK:64:ASN:HB3   | 1.94                     | 0.48              |
| 37:CD:59:LEU:CD1   | 37:CD:67:ARG:NH1   | 2.77                     | 0.48              |
| 39:CF:8:ILE:O      | 39:CF:12:VAL:HG23  | 2.14                     | 0.48              |
| 44:CK:20:SER:O     | 44:CK:24:ARG:HG2   | 2.13                     | 0.48              |
| 46:CM:444:A:N6     | 46:CM:459:G:H21    | 2.11                     | 0.48              |
| 46:CM:521:G:H5'    | 71:DL:60:PHE:O     | 2.13                     | 0.48              |
| 46:CM:741:A:H5'    | 51:CR:16:SER:CB    | 2.43                     | 0.48              |
| 46:CM:1227:A:O2'   | 46:CM:1229:A:OP1   | 2.30                     | 0.48              |
| 46:CM:1468:C:H5''  | 46:CM:1508:G:N2    | 2.23                     | 0.48              |
| 46:CM:1725:U:H2'   | 46:CM:1726:C:C6    | 2.49                     | 0.48              |
| 46:CM:1776:G:H5'   | 73:DN:17:HIS:CD2   | 2.48                     | 0.48              |
| 54:CU:41:SER:O     | 54:CU:57:PHE:HB2   | 2.14                     | 0.48              |
| 54:CU:166:GLN:HG3  | 54:CU:179:PHE:CD2  | 2.48                     | 0.48              |
| 59:CZ:48:ALA:O     | 59:CZ:122:VAL:HG21 | 2.14                     | 0.48              |
| 59:CZ:76:GLU:O     | 59:CZ:80:ASN:ND2   | 2.47                     | 0.48              |
| 59:CZ:138:GLU:HA   | 59:CZ:142:GLN:OE1  | 2.13                     | 0.48              |
| 69:DJ:7:LEU:HD11   | 69:DJ:37:PHE:CD2   | 2.44                     | 0.48              |
| 79:DT:254:THR:HG23 | 79:DT:285:GLU:CD   | 2.39                     | 0.48              |
| 81:P0:101:VAL:HG23 | 81:P0:102:SER:N    | 2.28                     | 0.48              |
| 1:1:246:U:H2'      | 1:1:247:C:C6       | 2.49                     | 0.48              |
| 1:1:291:C:H2'      | 1:1:292:U:C6       | 2.49                     | 0.48              |
| 1:1:961:A:O2'      | 29:AB:44:ASN:HB2   | 2.14                     | 0.48              |
| 1:1:1705:C:C2      | 1:1:1706:C:C5      | 3.02                     | 0.48              |
| 1:1:3025:G:H2'     | 1:1:3026:U:C6      | 2.49                     | 0.48              |
| 1:1:3166:A:H2'     | 1:1:3167:G:C8      | 2.48                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:j:80:GLU:HG3     | 44:AQ:66:GLY:HA2   | 1.94                     | 0.48              |
| 46:B:485:G:C2      | 46:B:486:G:C8      | 3.02                     | 0.48              |
| 46:B:1477:U:H4'    | 46:B:1478:A:H5'    | 1.95                     | 0.48              |
| 46:B:1498:G:H2'    | 46:B:1499:G:H8     | 1.77                     | 0.48              |
| 51:G:123:LEU:HD21  | 51:G:236:TRP:HB2   | 1.96                     | 0.48              |
| 53:I:182:GLN:HE21  | 53:I:186:ARG:HG3   | 1.79                     | 0.48              |
| 62:R:97:TYR:CE1    | 62:R:102:PHE:CE1   | 3.01                     | 0.48              |
| 75:e:18:ARG:CD     | 75:e:26:THR:HG22   | 2.44                     | 0.48              |
| 1:AS:725:G:H22     | 19:BL:139:ILE:HB   | 1.77                     | 0.48              |
| 1:AS:883:G:H2'     | 1:AS:884:A:C8      | 2.49                     | 0.48              |
| 1:AS:2385:C:H2'    | 1:AS:2386:U:C6     | 2.48                     | 0.48              |
| 1:AS:3193:C:H4'    | 1:AS:3194:G:O5'    | 2.14                     | 0.48              |
| 2:AT:71:U:O2'      | 2:AT:72:A:H5'      | 2.14                     | 0.48              |
| 5:AX:83:PRO:O      | 5:AX:165:GLN:NE2   | 2.33                     | 0.48              |
| 10:BC:45:ARG:O     | 26:BS:28:THR:HA    | 2.14                     | 0.48              |
| 10:BC:68:LEU:HB3   | 10:BC:238:ILE:HB   | 1.94                     | 0.48              |
| 13:BF:6:GLN:OE1    | 13:BF:6:GLN:N      | 2.47                     | 0.48              |
| 23:BP:92:ILE:HG22  | 23:BP:95:TRP:HZ3   | 1.79                     | 0.48              |
| 28:BU:3:LYS:HE3    | 28:BU:30:ASP:CG    | 2.39                     | 0.48              |
| 28:BU:14:VAL:HB    | 35:CB:86:LYS:HG3   | 1.96                     | 0.48              |
| 46:CM:79:C:H1'     | 53:CT:174:LYS:HB2  | 1.95                     | 0.48              |
| 46:CM:744:U:C2     | 46:CM:745:A:C8     | 3.02                     | 0.48              |
| 46:CM:1289:G:H5'   | 46:CM:1307:A:OP2   | 2.14                     | 0.48              |
| 46:CM:1741:A:C5    | 86:CM:1822:GET:H21 | 2.49                     | 0.48              |
| 47:CN:48:ILE:HG21  | 47:CN:161:PRO:HB2  | 1.96                     | 0.48              |
| 48:CO:53:GLY:O     | 48:CO:54:LEU:HB3   | 2.14                     | 0.48              |
| 50:CQ:158:MET:SD   | 50:CQ:188:LYS:HD2  | 2.54                     | 0.48              |
| 51:CR:104:ASP:HB3  | 51:CR:110:ALA:HB2  | 1.94                     | 0.48              |
| 51:CR:192:VAL:HG23 | 51:CR:244:GLY:HA3  | 1.96                     | 0.48              |
| 54:CU:47:VAL:CG2   | 54:CU:48:ASN:H     | 2.26                     | 0.48              |
| 61:DB:47:ARG:HG3   | 61:DB:48:ASP:OD1   | 2.13                     | 0.48              |
| 79:DT:50:GLY:HA3   | 79:DT:54:GLN:O     | 2.13                     | 0.48              |
| 1:1:28:C:OP1       | 16:v:189:HIS:HB2   | 2.14                     | 0.48              |
| 1:1:437:G:N2       | 1:1:620:A:H62      | 2.11                     | 0.48              |
| 1:1:486:C:H2'      | 1:1:487:C:C6       | 2.49                     | 0.48              |
| 1:1:1165:A:H4'     | 9:o:216:LYS:HD2    | 1.96                     | 0.48              |
| 1:1:1218:G:OP1     | 81:P0:55:LYS:HE2   | 2.14                     | 0.48              |
| 1:1:2201:A:O3'     | 37:AJ:73:LYS:NZ    | 2.44                     | 0.48              |
| 1:1:2738:U:H2'     | 1:1:2739:U:C6      | 2.49                     | 0.48              |
| 2:3:16:U:H2'       | 2:3:17:A:C8        | 2.49                     | 0.48              |
| 2:3:70:A:H2'       | 2:3:71:U:H6        | 1.78                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:o:108:GLN:HG3   | 9:o:111:ALA:HB2    | 1.96                     | 0.48              |
| 34:AG:35:VAL:HG12 | 34:AG:79:GLY:HA3   | 1.96                     | 0.48              |
| 46:B:17:C:H2'     | 46:B:18:C:H6       | 1.77                     | 0.48              |
| 46:B:673:A:H8     | 46:B:673:A:O5'     | 1.96                     | 0.48              |
| 46:B:684:C:H2'    | 46:B:685:C:H6      | 1.79                     | 0.48              |
| 46:B:1369:G:O2'   | 46:B:1370:A:H8     | 1.97                     | 0.48              |
| 52:H:32:ASP:OD1   | 52:H:33:VAL:N      | 2.46                     | 0.48              |
| 65:U:63:GLN:O     | 65:U:67:GLU:HG3    | 2.14                     | 0.48              |
| 69:Y:15:ASN:ND2   | 69:Y:72:CYS:O      | 2.32                     | 0.48              |
| 1:AS:259:C:H2'    | 1:AS:260:C:C6      | 2.49                     | 0.48              |
| 1:AS:539:G:H2'    | 1:AS:540:C:O4'     | 2.14                     | 0.48              |
| 1:AS:922:A:H2'    | 1:AS:923:C:C6      | 2.49                     | 0.48              |
| 1:AS:962:U:H2'    | 1:AS:963:A:C8      | 2.48                     | 0.48              |
| 1:AS:2236:U:C2    | 1:AS:2237:A:C8     | 3.02                     | 0.48              |
| 1:AS:2279:U:H2'   | 1:AS:2280:G:H8     | 1.79                     | 0.48              |
| 1:AS:3259:A:H2'   | 1:AS:3260:A:O4'    | 2.14                     | 0.48              |
| 3:AU:40:A:H2'     | 3:AU:41:A:C8       | 2.49                     | 0.48              |
| 3:AU:154:C:H5''   | 10:BC:182:LYS:HG2  | 1.95                     | 0.48              |
| 3:AU:156:U:O2'    | 3:AU:157:U:P       | 2.72                     | 0.48              |
| 10:BC:229:GLU:HA  | 10:BC:232:LYS:HD2  | 1.96                     | 0.48              |
| 11:BD:47:LYS:NZ   | 15:BH:3:SER:HA     | 2.29                     | 0.48              |
| 20:BM:134:HIS:HE1 | 20:BM:136:ARG:HB3  | 1.77                     | 0.48              |
| 37:CD:56:LEU:O    | 37:CD:60:ILE:HG13  | 2.14                     | 0.48              |
| 39:CF:58:ASP:HB3  | 39:CF:61:LYS:CB    | 2.44                     | 0.48              |
| 46:CM:485:G:N2    | 46:CM:486:G:H1'    | 2.29                     | 0.48              |
| 46:CM:558:U:H2'   | 46:CM:559:G:H8     | 1.79                     | 0.48              |
| 46:CM:696:U:OP1   | 46:CM:696:U:H6     | 1.95                     | 0.48              |
| 46:CM:1233:C:C2   | 46:CM:1234:U:H5    | 2.31                     | 0.48              |
| 50:CQ:109:LYS:HE3 | 50:CQ:114:LEU:HD22 | 1.95                     | 0.48              |
| 52:CS:25:LEU:HG   | 52:CS:29:ILE:HG12  | 1.96                     | 0.48              |
| 52:CS:27:THR:CG2  | 52:CS:28:THR:N     | 2.76                     | 0.48              |
| 54:CU:65:ALA:HA   | 54:CU:68:LYS:NZ    | 2.29                     | 0.48              |
| 54:CU:69:VAL:HA   | 54:CU:72:ARG:HB2   | 1.95                     | 0.48              |
| 65:DF:25:ARG:HB3  | 65:DF:25:ARG:HH11  | 1.78                     | 0.48              |
| 71:DL:56:SER:HB3  | 71:DL:74:LEU:HD11  | 1.94                     | 0.48              |
| 79:DT:107:HIS:CE1 | 79:DT:129:ASP:HB2  | 2.47                     | 0.48              |
| 79:DT:148:HIS:ND1 | 79:DT:170:SER:HB3  | 2.29                     | 0.48              |
| 79:DT:226:LYS:CD  | 79:DT:227:THR:H    | 2.05                     | 0.48              |
| 1:1:61:A:H2'      | 1:1:62:A:C8        | 2.48                     | 0.48              |
| 1:1:234:A:H4'     | 38:AK:86:GLN:HG2   | 1.96                     | 0.48              |
| 1:1:1187:U:OP2    | 17:w:50:ARG:HD2    | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:2183:U:O4      | 1:1:2216:G:N1      | 2.47                     | 0.48              |
| 1:1:3013:U:H2'     | 1:1:3014:U:C6      | 2.49                     | 0.48              |
| 9:o:100:VAL:HG13   | 9:o:124:LEU:HD22   | 1.96                     | 0.48              |
| 13:s:88:GLU:HB3    | 62:R:13:LYS:HE3    | 1.95                     | 0.48              |
| 18:x:29:THR:HA     | 18:x:32:THR:HG22   | 1.96                     | 0.48              |
| 28:AA:119:GLU:O    | 28:AA:123:GLN:HG2  | 2.13                     | 0.48              |
| 40:AM:27:ILE:O     | 40:AM:33:ASN:ND2   | 2.47                     | 0.48              |
| 46:B:767:G:O2'     | 46:B:768:C:H6      | 1.97                     | 0.48              |
| 46:B:809:G:H2'     | 46:B:810:U:C6      | 2.49                     | 0.48              |
| 46:B:1220:C:N4     | 78:h:177:MET:HE1   | 2.29                     | 0.48              |
| 56:L:106:GLU:HA    | 56:L:111:THR:HG21  | 1.96                     | 0.48              |
| 59:O:27:ALA:HB1    | 59:O:132:GLU:HG2   | 1.95                     | 0.48              |
| 1:AS:708:A:H4'     | 29:BV:58:MET:HE2   | 1.96                     | 0.48              |
| 1:AS:1113:G:OP1    | 30:BW:4:SER:HB2    | 2.14                     | 0.48              |
| 1:AS:1468:U:H2'    | 1:AS:1469:G:H8     | 1.78                     | 0.48              |
| 1:AS:1496:G:H2'    | 1:AS:1497:U:O4'    | 2.13                     | 0.48              |
| 1:AS:1634:A:H5''   | 35:CB:82:ALA:HB2   | 1.95                     | 0.48              |
| 1:AS:2397:A:H2'    | 1:AS:2398:C:C6     | 2.49                     | 0.48              |
| 6:AY:161:THR:HG22  | 6:AY:215:GLY:HA3   | 1.95                     | 0.48              |
| 19:BL:125:ASP:OD1  | 19:BL:126:GLN:N    | 2.47                     | 0.48              |
| 39:CF:38:PHE:CZ    | 39:CF:40:GLN:HB3   | 2.49                     | 0.48              |
| 39:CF:58:ASP:CG    | 39:CF:61:LYS:H     | 2.22                     | 0.48              |
| 46:CM:302:U:H2'    | 46:CM:303:C:H6     | 1.77                     | 0.48              |
| 46:CM:325:U:H2'    | 46:CM:326:A:H8     | 1.79                     | 0.48              |
| 46:CM:446:C:H2'    | 46:CM:447:C:H6     | 1.79                     | 0.48              |
| 46:CM:1338:U:H1'   | 46:CM:1358:G:H21   | 1.79                     | 0.48              |
| 46:CM:1455:A:H2'   | 46:CM:1456:C:C6    | 2.49                     | 0.48              |
| 48:CO:168:MET:HA   | 48:CO:197:ILE:CD1  | 2.42                     | 0.48              |
| 48:CO:214:LYS:HE3  | 48:CO:214:LYS:HB2  | 1.48                     | 0.48              |
| 52:CS:47:SER:O     | 52:CS:130:ILE:HD11 | 2.14                     | 0.48              |
| 57:CX:32:HIS:HB2   | 57:CX:39:ASN:HA    | 1.96                     | 0.48              |
| 62:DC:61:ARG:HD3   | 62:DC:88:GLU:HG2   | 1.96                     | 0.48              |
| 73:DN:12:LYS:HA    | 73:DN:15:ARG:HH12  | 1.79                     | 0.48              |
| 79:DT:167:ILE:HD12 | 79:DT:167:ILE:O    | 2.14                     | 0.48              |
| 1:1:122:A:OP1      | 10:p:106:LYS:NZ    | 2.42                     | 0.47              |
| 1:1:430:G:H2'      | 1:1:431:A:H8       | 1.79                     | 0.47              |
| 1:1:548:G:H2'      | 1:1:549:U:H6       | 1.79                     | 0.47              |
| 1:1:762:U:H4'      | 1:1:763:U:O4'      | 2.13                     | 0.47              |
| 1:1:815:U:H2'      | 1:1:816:A:H8       | 1.79                     | 0.47              |
| 1:1:845:C:H2'      | 1:1:846:U:C6       | 2.48                     | 0.47              |
| 1:1:964:G:H2'      | 1:1:965:C:H6       | 1.78                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:972:U:H2'     | 1:1:973:C:O4'      | 2.14                     | 0.47              |
| 1:1:1024:U:H4'    | 1:1:1024:U:OP1     | 2.14                     | 0.47              |
| 1:1:1757:A:O2'    | 1:1:1759:U:OP2     | 2.23                     | 0.47              |
| 1:1:1909:A:N3     | 1:1:2098:A:H2'     | 2.29                     | 0.47              |
| 1:1:2130:A:H2'    | 1:1:2131:U:C6      | 2.48                     | 0.47              |
| 1:1:2874:A:H2'    | 1:1:2875:A:O4'     | 2.14                     | 0.47              |
| 7:m:60:ILE:HB     | 7:m:80:ALA:HB2     | 1.96                     | 0.47              |
| 15:u:20:LEU:HD21  | 15:u:23:ASN:CA     | 2.43                     | 0.47              |
| 17:w:62:ALA:HA    | 17:w:71:PRO:HD2    | 1.96                     | 0.47              |
| 21:0:44:PHE:O     | 21:0:48:LEU:HD12   | 2.14                     | 0.47              |
| 31:AD:12:ILE:O    | 31:AD:15:LYS:N     | 2.47                     | 0.47              |
| 46:B:1757:U:H2'   | 46:B:1758:U:C6     | 2.49                     | 0.47              |
| 63:S:34:PRO:HD2   | 66:V:7:ARG:O       | 2.14                     | 0.47              |
| 65:U:62:THR:HG23  | 65:U:65:GLU:H      | 1.78                     | 0.47              |
| 72:b:65:LEU:HD23  | 72:b:71:ILE:HD11   | 1.96                     | 0.47              |
| 1:AS:268:A:C4     | 16:BI:12:ARG:HG2   | 2.48                     | 0.47              |
| 1:AS:362:U:O4     | 38:CE:24:ARG:NH2   | 2.46                     | 0.47              |
| 1:AS:394:G:N1     | 1:AS:397:A:OP2     | 2.46                     | 0.47              |
| 1:AS:1358:C:H2'   | 1:AS:1359:A:C8     | 2.49                     | 0.47              |
| 1:AS:1758:U:H5    | 1:AS:1759:U:HO2'   | 1.62                     | 0.47              |
| 1:AS:3044:C:H2'   | 1:AS:3045:A:O4'    | 2.14                     | 0.47              |
| 1:AS:3201:U:H1'   | 1:AS:3217:G:N2     | 2.29                     | 0.47              |
| 2:AT:77:G:H3'     | 21:BN:46:GLN:O     | 2.14                     | 0.47              |
| 5:AX:103:THR:HG21 | 5:AX:147:GLU:HB3   | 1.96                     | 0.47              |
| 9:BB:39:ARG:HA    | 9:BB:42:ILE:HG12   | 1.95                     | 0.47              |
| 10:BC:172:LYS:HA  | 10:BC:224:ILE:HD11 | 1.95                     | 0.47              |
| 14:BG:48:PRO:HB3  | 36:CC:117:ALA:HB2  | 1.95                     | 0.47              |
| 39:CF:40:GLN:CB   | 39:CF:57:ASN:HA    | 2.37                     | 0.47              |
| 46:CM:701:G:N2    | 46:CM:721:C:O2     | 2.47                     | 0.47              |
| 46:CM:913:U:H3'   | 46:CM:929:A:O2'    | 2.14                     | 0.47              |
| 46:CM:1193:A:H8   | 46:CM:1254:U:H6    | 1.62                     | 0.47              |
| 46:CM:1335:U:H2'  | 46:CM:1336:G:H8    | 1.78                     | 0.47              |
| 46:CM:1716:C:H2'  | 46:CM:1717:A:O4'   | 2.14                     | 0.47              |
| 48:CO:51:SER:HB2  | 48:CO:57:ALA:HB2   | 1.96                     | 0.47              |
| 59:CZ:32:LEU:HD13 | 59:CZ:41:LEU:HD21  | 1.96                     | 0.47              |
| 79:DT:101:THR:O   | 79:DT:102:GLN:C    | 2.56                     | 0.47              |
| 79:DT:209:ALA:CB  | 79:DT:249:LEU:HD21 | 2.43                     | 0.47              |
| 79:DT:252:ALA:HB1 | 79:DT:286:ALA:HB3  | 1.96                     | 0.47              |
| 79:DT:258:LYS:HG3 | 79:DT:267:LEU:CD1  | 2.44                     | 0.47              |
| 1:1:127:G:OP2     | 36:AI:74:LYS:NZ    | 2.46                     | 0.47              |
| 1:1:1240:A:O2'    | 1:1:1244:C:N4      | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:2509:C:C4      | 1:1:2510:U:C4      | 3.02                     | 0.47              |
| 1:1:2894:G:H1'     | 1:1:2923:G:N3      | 2.29                     | 0.47              |
| 14:t:24:VAL:HG22   | 16:v:199:LEU:HB2   | 1.95                     | 0.47              |
| 18:x:18:ARG:NH1    | 18:x:147:GLU:OE1   | 2.46                     | 0.47              |
| 25:7:116:LYS:HG2   | 25:7:117:LYS:HE3   | 1.96                     | 0.47              |
| 46:B:739:A:H5''    | 46:B:740:A:H5'     | 1.96                     | 0.47              |
| 46:B:1414:G:C2'    | 46:B:1415:G:H5'    | 2.44                     | 0.47              |
| 48:D:103:LEU:HB3   | 48:D:215:VAL:HB    | 1.96                     | 0.47              |
| 49:E:107:GLY:HA3   | 49:E:131:ILE:HG12  | 1.96                     | 0.47              |
| 59:O:38:HIS:O      | 59:O:39:ASP:C      | 2.56                     | 0.47              |
| 76:f:39:CYS:CB     | 76:f:42:CYS:H      | 2.27                     | 0.47              |
| 78:h:180:ARG:HA    | 78:h:190:LEU:O     | 2.14                     | 0.47              |
| 79:AR:133:LYS:HE2  | 79:AR:144:THR:HG22 | 1.96                     | 0.47              |
| 1:AS:157:G:H2'     | 1:AS:158:A:H8      | 1.78                     | 0.47              |
| 1:AS:291:C:H2'     | 1:AS:292:U:C6      | 2.49                     | 0.47              |
| 1:AS:393:U:H2'     | 1:AS:394:G:O4'     | 2.14                     | 0.47              |
| 1:AS:629:A:H2'     | 1:AS:630:G:C8      | 2.49                     | 0.47              |
| 1:AS:1034:U:O3'    | 7:AZ:5:LYS:HA      | 2.14                     | 0.47              |
| 1:AS:2388:U:H3     | 1:AS:2773:A:H2     | 1.60                     | 0.47              |
| 1:AS:2680:C:H2'    | 1:AS:2681:C:H6     | 1.80                     | 0.47              |
| 5:AX:66:LYS:NZ     | 24:BQ:9:ASN:H      | 2.12                     | 0.47              |
| 9:BB:198:ASN:HD22  | 9:BB:198:ASN:C     | 2.20                     | 0.47              |
| 11:BD:100:ASN:HB3  | 11:BD:115:ARG:HB2  | 1.96                     | 0.47              |
| 26:BS:70:GLU:HG2   | 26:BS:74:LYS:NZ    | 2.28                     | 0.47              |
| 26:BS:105:VAL:HG23 | 26:BS:130:TYR:CG   | 2.48                     | 0.47              |
| 46:CM:82:U:H2'     | 46:CM:83:G:O4'     | 2.14                     | 0.47              |
| 46:CM:116:U:H2'    | 46:CM:117:U:C6     | 2.47                     | 0.47              |
| 46:CM:398:A:H5''   | 55:CV:25:ARG:HA    | 1.96                     | 0.47              |
| 46:CM:657:C:N4     | 46:CM:667:A:H62    | 2.11                     | 0.47              |
| 46:CM:816:U:H2'    | 46:CM:817:U:C6     | 2.49                     | 0.47              |
| 46:CM:852:G:H1     | 46:CM:946:U:H3     | 1.61                     | 0.47              |
| 46:CM:1070:G:H2'   | 46:CM:1072:A:OP2   | 2.14                     | 0.47              |
| 46:CM:1220:C:H3'   | 46:CM:1221:A:H8    | 1.79                     | 0.47              |
| 46:CM:1634:U:H2'   | 46:CM:1635:A:C8    | 2.50                     | 0.47              |
| 48:CO:134:VAL:HB   | 48:CO:219:LYS:HB3  | 1.96                     | 0.47              |
| 59:CZ:107:ASP:OD1  | 59:CZ:108:ARG:N    | 2.37                     | 0.47              |
| 79:DT:33:LEU:O     | 79:DT:45:TRP:N     | 2.47                     | 0.47              |
| 79:DT:63:LYS:O     | 79:DT:93:TRP:HZ3   | 1.97                     | 0.47              |
| 82:12:104:ILE:HD12 | 82:12:142:ARG:O    | 2.14                     | 0.47              |
| 1:1:516:U:OP1      | 6:l:352:PRO:HD2    | 2.14                     | 0.47              |
| 1:1:942:U:H2'      | 1:1:943:G:H8       | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1012:U:H4'    | 1:1:1013:U:H4'    | 1.95                     | 0.47              |
| 1:1:1153:G:H2'    | 1:1:1154:A:O4'    | 2.15                     | 0.47              |
| 1:1:1216:U:P      | 1:1:1218:G:H5'    | 2.55                     | 0.47              |
| 1:1:2197:A:H2'    | 1:1:2198:A:C8     | 2.48                     | 0.47              |
| 2:3:1:G:C4        | 7:m:266:LYS:HA    | 2.49                     | 0.47              |
| 2:3:3:U:H2'       | 2:3:4:U:C6        | 2.49                     | 0.47              |
| 12:r:86:HIS:HB3   | 12:r:139:ARG:CG   | 2.44                     | 0.47              |
| 46:B:252:A:H2'    | 46:B:253:U:C6     | 2.49                     | 0.47              |
| 46:B:289:G:H2'    | 46:B:290:U:C5     | 2.49                     | 0.47              |
| 46:B:333:U:O2'    | 58:N:130:PRO:O    | 2.25                     | 0.47              |
| 46:B:1485:G:H5''  | 66:V:72:GLY:HA3   | 1.96                     | 0.47              |
| 51:G:150:PRO:O    | 53:I:208:TYR:HE1  | 1.96                     | 0.47              |
| 1:AS:73:G:H8      | 14:BG:104:LYS:NZ  | 2.12                     | 0.47              |
| 1:AS:200:A:H2'    | 1:AS:201:G:C8     | 2.49                     | 0.47              |
| 1:AS:493:A:O2'    | 1:AS:3238:A:N1    | 2.35                     | 0.47              |
| 1:AS:520:G:C4     | 1:AS:521:G:C8     | 3.03                     | 0.47              |
| 1:AS:1226:G:H3'   | 1:AS:1227:A:C8    | 2.48                     | 0.47              |
| 1:AS:1810:A:H4'   | 1:AS:1811:U:O4'   | 2.14                     | 0.47              |
| 1:AS:2927:U:H2'   | 1:AS:2928:A:O4'   | 2.14                     | 0.47              |
| 1:AS:2983:A:N1    | 1:AS:3015:C:O2'   | 2.38                     | 0.47              |
| 1:AS:3129:C:H2'   | 1:AS:3130:C:H6    | 1.79                     | 0.47              |
| 1:AS:3139:U:N3    | 1:AS:3247:A:C2    | 2.82                     | 0.47              |
| 5:AX:152:LYS:HA   | 5:AX:188:VAL:HG12 | 1.97                     | 0.47              |
| 10:BC:134:LYS:HG3 | 10:BC:139:HIS:HE1 | 1.79                     | 0.47              |
| 18:BK:32:THR:HG21 | 18:BK:87:SER:HB3  | 1.95                     | 0.47              |
| 28:BU:84:ARG:HG2  | 28:BU:84:ARG:HH11 | 1.79                     | 0.47              |
| 28:BU:101:LEU:HA  | 28:BU:107:ARG:HG2 | 1.95                     | 0.47              |
| 46:CM:265:U:H2'   | 46:CM:266:C:H6    | 1.79                     | 0.47              |
| 46:CM:382:G:H2'   | 46:CM:383:A:C8    | 2.48                     | 0.47              |
| 46:CM:478:G:H1    | 46:CM:506:U:H3    | 1.62                     | 0.47              |
| 46:CM:690:C:H2'   | 46:CM:691:U:H6    | 1.78                     | 0.47              |
| 46:CM:770:C:OP1   | 46:CM:770:C:H6    | 1.97                     | 0.47              |
| 46:CM:1652:U:O2   | 46:CM:1723:G:N2   | 2.42                     | 0.47              |
| 47:CN:41:ARG:CD   | 47:CN:47:ILE:HD11 | 2.45                     | 0.47              |
| 48:CO:79:HIS:HA   | 48:CO:81:TYR:CE1  | 2.49                     | 0.47              |
| 52:CS:43:PHE:CG   | 52:CS:115:LYS:HD3 | 2.48                     | 0.47              |
| 53:CT:74:ARG:NH1  | 53:CT:96:SER:OG   | 2.42                     | 0.47              |
| 59:CZ:77:ALA:CB   | 78:DS:156:VAL:HB  | 2.44                     | 0.47              |
| 65:DF:46:VAL:HG11 | 65:DF:73:MET:HG2  | 1.96                     | 0.47              |
| 73:DN:35:ALA:O    | 73:DN:37:LYS:HD3  | 2.14                     | 0.47              |
| 78:DS:181:GLN:OE1 | 78:DS:182:TYR:N   | 2.47                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:DT:82:LEU:HG    | 79:DT:92:LEU:HD13 | 1.95                     | 0.47              |
| 1:1:1041:C:OP1     | 12:r:133:GLN:NE2  | 2.45                     | 0.47              |
| 1:1:1632:C:H4'     | 28:AA:74:LEU:O    | 2.15                     | 0.47              |
| 1:1:2081:U:H2'     | 1:1:2082:A:C8     | 2.48                     | 0.47              |
| 1:1:2279:U:H2'     | 1:1:2280:G:H8     | 1.79                     | 0.47              |
| 1:1:2664:A:H4'     | 45:i:42:ALA:HB1   | 1.96                     | 0.47              |
| 1:1:2734:A:H2'     | 1:1:2735:U:H6     | 1.80                     | 0.47              |
| 7:m:98:ALA:HB1     | 7:m:162:VAL:HG23  | 1.96                     | 0.47              |
| 8:n:146:LEU:O      | 8:n:150:LYS:HG2   | 2.15                     | 0.47              |
| 25:7:13:ILE:HG12   | 25:7:32:GLN:HB2   | 1.96                     | 0.47              |
| 26:8:43:SER:O      | 26:8:43:SER:OG    | 2.31                     | 0.47              |
| 46:B:74:U:O2'      | 46:B:76:A:OP1     | 2.25                     | 0.47              |
| 46:B:1242:U:O2     | 46:B:1242:U:H2'   | 2.13                     | 0.47              |
| 46:B:1670:U:O2'    | 46:B:1671:G:O5'   | 2.27                     | 0.47              |
| 48:D:62:LYS:HZ2    | 48:D:90:GLU:HA    | 1.79                     | 0.47              |
| 50:F:69:GLU:O      | 57:M:20:VAL:HG11  | 2.14                     | 0.47              |
| 54:J:137:ARG:NH2   | 69:Y:49:GLU:OE1   | 2.42                     | 0.47              |
| 57:M:62:GLN:CD     | 76:f:25:SER:HB3   | 2.39                     | 0.47              |
| 59:O:63:CYS:HB3    | 59:O:97:LEU:HD11  | 1.96                     | 0.47              |
| 59:O:132:GLU:OE2   | 59:O:136:LEU:HD13 | 2.15                     | 0.47              |
| 78:h:178:LYS:HB3   | 78:h:179:ASP:H    | 1.48                     | 0.47              |
| 79:AR:42:LEU:HD11  | 79:AR:83:SER:HB3  | 1.96                     | 0.47              |
| 1:AS:79:G:H2'      | 1:AS:80:C:H6      | 1.78                     | 0.47              |
| 1:AS:240:C:H5'     | 1:AS:241:C:H5''   | 1.95                     | 0.47              |
| 1:AS:638:U:H2'     | 1:AS:639:C:C6     | 2.49                     | 0.47              |
| 1:AS:787:A:H2'     | 1:AS:788:G:H8     | 1.79                     | 0.47              |
| 1:AS:792:U:H2'     | 1:AS:793:U:C6     | 2.49                     | 0.47              |
| 1:AS:1165:A:H2'    | 1:AS:1166:A:C8    | 2.49                     | 0.47              |
| 1:AS:1756:A:C2     | 1:AS:1759:U:H5    | 2.33                     | 0.47              |
| 1:AS:2090:U:H4'    | 1:AS:2091:A:O5'   | 2.13                     | 0.47              |
| 1:AS:2801:U:C2     | 1:AS:2802:G:C8    | 3.02                     | 0.47              |
| 1:AS:3285:A:H2'    | 1:AS:3286:C:H6    | 1.80                     | 0.47              |
| 3:AU:19:C:H2'      | 3:AU:20:U:C6      | 2.49                     | 0.47              |
| 6:AY:296:VAL:O     | 6:AY:300:VAL:HG13 | 2.14                     | 0.47              |
| 23:BP:17:VAL:O     | 23:BP:63:LYS:HA   | 2.15                     | 0.47              |
| 28:BU:134:LEU:HD23 | 28:BU:136:PHE:CE1 | 2.49                     | 0.47              |
| 36:CC:9:LEU:CD2    | 36:CC:54:VAL:HG22 | 2.45                     | 0.47              |
| 46:CM:75:U:H2'     | 46:CM:76:A:N3     | 2.29                     | 0.47              |
| 46:CM:446:C:H2'    | 46:CM:447:C:C6    | 2.50                     | 0.47              |
| 46:CM:584:G:H2'    | 46:CM:585:C:C6    | 2.49                     | 0.47              |
| 46:CM:1273:G:N7    | 46:CM:1299:U:O2'  | 2.39                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:CO:30:PHE:HE1  | 48:CO:46:THR:OG1  | 1.97                     | 0.47              |
| 54:CU:51:LYS:C    | 54:CU:52:LYS:HG3  | 2.39                     | 0.47              |
| 78:DS:147:TYR:O   | 78:DS:159:LEU:N   | 2.36                     | 0.47              |
| 79:DT:284:PRO:HG2 | 79:DT:304:ASP:HB3 | 1.95                     | 0.47              |
| 1:1:72:A:C5       | 37:AJ:14:ARG:HD2  | 2.49                     | 0.47              |
| 1:1:755:U:H2'     | 1:1:756:G:O4'     | 2.15                     | 0.47              |
| 11:q:92:PHE:HB2   | 11:q:142:ASP:HB3  | 1.96                     | 0.47              |
| 13:s:46:VAL:HG12  | 45:i:35:SER:CB    | 2.45                     | 0.47              |
| 18:x:19:GLY:HA3   | 18:x:22:LEU:HD11  | 1.95                     | 0.47              |
| 25:7:81:ALA:HB3   | 53:I:130:PRO:HB3  | 1.96                     | 0.47              |
| 46:B:15:U:H2'     | 46:B:16:G:O4'     | 2.14                     | 0.47              |
| 46:B:220:A:N6     | 46:B:824:U:O2     | 2.47                     | 0.47              |
| 46:B:787:A:O2'    | 54:J:100:ARG:NE   | 2.47                     | 0.47              |
| 46:B:975:C:H1'    | 61:Q:122:ARG:HG2  | 1.96                     | 0.47              |
| 46:B:1132:A:H2'   | 46:B:1133:C:H6    | 1.79                     | 0.47              |
| 48:D:66:PHE:CE1   | 61:Q:29:SER:HB3   | 2.50                     | 0.47              |
| 48:D:129:THR:OG1  | 48:D:131:ASP:OD1  | 2.30                     | 0.47              |
| 1:AS:158:A:H2'    | 1:AS:159:A:H8     | 1.80                     | 0.47              |
| 1:AS:787:A:H2'    | 1:AS:788:G:C8     | 2.49                     | 0.47              |
| 1:AS:912:G:N1     | 4:AW:207:VAL:HG11 | 2.29                     | 0.47              |
| 1:AS:1077:U:H5'   | 1:AS:1078:U:H5    | 1.80                     | 0.47              |
| 1:AS:1114:C:OP2   | 30:BW:5:LYS:HD3   | 2.15                     | 0.47              |
| 1:AS:1561:U:H5''  | 1:AS:1561:U:C6    | 2.49                     | 0.47              |
| 1:AS:2287:A:N3    | 1:AS:2933:G:O2'   | 2.38                     | 0.47              |
| 1:AS:3143:G:C2    | 34:CA:96:ALA:HB2  | 2.50                     | 0.47              |
| 1:AS:3182:C:O4'   | 1:AS:3231:G:N2    | 2.47                     | 0.47              |
| 4:AW:98:VAL:HA    | 4:AW:166:ILE:HG22 | 1.96                     | 0.47              |
| 10:BC:86:ASN:O    | 10:BC:90:GLN:HG3  | 2.14                     | 0.47              |
| 20:BM:39:SER:HA   | 20:BM:42:ARG:HH11 | 1.78                     | 0.47              |
| 20:BM:165:ARG:NH1 | 46:CM:835:A:OP1   | 2.47                     | 0.47              |
| 22:BO:116:LYS:O   | 22:BO:120:LYS:HG3 | 2.14                     | 0.47              |
| 26:BS:109:TYR:HE1 | 26:BS:125:ARG:HD2 | 1.78                     | 0.47              |
| 39:CF:46:ARG:NH1  | 39:CF:47:GLY:H    | 2.13                     | 0.47              |
| 45:CL:126:GLU:O   | 45:CL:130:GLU:HG2 | 2.15                     | 0.47              |
| 46:CM:445:U:OP1   | 51:CR:49:ARG:NH1  | 2.47                     | 0.47              |
| 46:CM:528:C:O2    | 71:DL:61:ARG:NH1  | 2.37                     | 0.47              |
| 46:CM:584:G:H2'   | 46:CM:585:C:H6    | 1.79                     | 0.47              |
| 46:CM:728:U:OP2   | 54:CU:103:ARG:HA  | 2.14                     | 0.47              |
| 46:CM:814:A:H2'   | 46:CM:814:A:OP2   | 2.15                     | 0.47              |
| 46:CM:1306:A:H4'  | 46:CM:1307:A:O5'  | 2.15                     | 0.47              |
| 46:CM:1414:G:H3'  | 46:CM:1414:G:OP2  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:CM:1520:C:H4'  | 46:CM:1526:G:O6   | 2.13                     | 0.47              |
| 46:CM:1529:G:N2   | 46:CM:1555:C:H1'  | 2.30                     | 0.47              |
| 47:CN:79:ARG:O    | 47:CN:83:GLN:HG3  | 2.13                     | 0.47              |
| 59:CZ:97:LEU:HD13 | 59:CZ:119:SER:CA  | 2.43                     | 0.47              |
| 71:DL:57:VAL:HB   | 71:DL:60:PHE:HE1  | 1.79                     | 0.47              |
| 79:DT:159:PRO:HG3 | 79:DT:203:PRO:HA  | 1.97                     | 0.47              |
| 81:P0:55:LYS:HG2  | 81:P0:56:ASN:N    | 2.30                     | 0.47              |
| 1:1:412:G:H2'     | 1:1:413:U:C6      | 2.50                     | 0.47              |
| 1:1:793:U:O2      | 14:t:12:ASN:ND2   | 2.47                     | 0.47              |
| 1:1:976:A:H2      | 1:1:1100:G:H21    | 1.61                     | 0.47              |
| 1:1:1391:G:O2'    | 3:4:18:U:O2       | 2.33                     | 0.47              |
| 1:1:1569:C:H2'    | 1:1:1570:A:C8     | 2.49                     | 0.47              |
| 1:1:1714:G:H2'    | 1:1:1715:G:C8     | 2.49                     | 0.47              |
| 1:1:1756:A:C2     | 1:1:1759:U:H5     | 2.33                     | 0.47              |
| 2:3:47:C:OP2      | 7:m:158:ARG:HD3   | 2.15                     | 0.47              |
| 8:n:53:TYR:CE1    | 8:n:62:LEU:HB3    | 2.49                     | 0.47              |
| 14:t:56:PRO:HG3   | 14:t:74:GLY:O     | 2.15                     | 0.47              |
| 46:B:125:U:OP1    | 53:I:201:GLN:NE2  | 2.41                     | 0.47              |
| 46:B:1654:A:H2'   | 46:B:1655:G:H8    | 1.80                     | 0.47              |
| 55:K:39:GLY:O     | 55:K:61:GLU:HG3   | 2.15                     | 0.47              |
| 61:Q:76:ILE:HB    | 61:Q:110:ILE:HG12 | 1.95                     | 0.47              |
| 1:AS:649:G:O2'    | 1:AS:1431:A:OP1   | 2.31                     | 0.47              |
| 1:AS:1377:A:H2'   | 1:AS:1378:G:C8    | 2.49                     | 0.47              |
| 1:AS:1696:G:H2'   | 1:AS:1697:C:C6    | 2.49                     | 0.47              |
| 1:AS:2397:A:H1'   | 1:AS:2776:A:O4'   | 2.15                     | 0.47              |
| 3:AU:45:C:H3'     | 40:CG:15:LYS:NZ   | 2.29                     | 0.47              |
| 3:AU:56:G:H5''    | 38:CE:68:LYS:NZ   | 2.30                     | 0.47              |
| 3:AU:139:U:H2'    | 3:AU:140:G:H8     | 1.79                     | 0.47              |
| 4:AW:117:GLU:OE2  | 4:AW:163:ARG:NH2  | 2.46                     | 0.47              |
| 17:BJ:2:SER:N     | 21:BN:161:LYS:HZ2 | 2.11                     | 0.47              |
| 26:BS:65:ALA:O    | 26:BS:85:GLN:N    | 2.43                     | 0.47              |
| 28:BU:108:GLU:CG  | 28:BU:112:LYS:HE3 | 2.45                     | 0.47              |
| 37:CD:73:LYS:HE3  | 37:CD:79:HIS:CB   | 2.40                     | 0.47              |
| 39:CF:38:PHE:CE1  | 39:CF:57:ASN:HB3  | 2.48                     | 0.47              |
| 46:CM:79:C:OP1    | 53:CT:172:ALA:HB3 | 2.15                     | 0.47              |
| 46:CM:849:U:P     | 69:DJ:28:ARG:HH12 | 2.38                     | 0.47              |
| 46:CM:953:U:H2'   | 46:CM:954:C:O4'   | 2.14                     | 0.47              |
| 46:CM:1245:U:H2'  | 46:CM:1246:G:C8   | 2.50                     | 0.47              |
| 46:CM:1431:G:C5   | 78:DS:131:LYS:HD2 | 2.50                     | 0.47              |
| 46:CM:1453:C:O2'  | 66:DG:88:PHE:O    | 2.19                     | 0.47              |
| 46:CM:1469:A:OP2  | 46:CM:1508:G:N2   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:CM:1774:C:H2'  | 46:CM:1775:G:H8   | 1.78                     | 0.47              |
| 48:CO:109:LYS:O   | 48:CO:113:LEU:HG  | 2.15                     | 0.47              |
| 54:CU:35:ARG:HB2  | 54:CU:36:PRO:HD3  | 1.96                     | 0.47              |
| 64:DE:99:GLN:HB3  | 64:DE:118:PRO:O   | 2.14                     | 0.47              |
| 67:DH:32:GLN:HB3  | 67:DH:108:GLU:HG2 | 1.94                     | 0.47              |
| 1:1:76:A:H5'      | 14:t:100:ARG:CZ   | 2.44                     | 0.47              |
| 1:1:259:C:H2'     | 1:1:260:C:H6      | 1.80                     | 0.47              |
| 1:1:532:U:H2'     | 1:1:533:G:H8      | 1.80                     | 0.47              |
| 1:1:582:G:H2'     | 1:1:583:A:H8      | 1.78                     | 0.47              |
| 1:1:729:C:H3'     | 1:1:730:A:H5''    | 1.97                     | 0.47              |
| 1:1:843:A:H2'     | 1:1:844:A:C8      | 2.49                     | 0.47              |
| 1:1:988:A:O2'     | 1:1:989:G:H5'     | 2.14                     | 0.47              |
| 1:1:989:G:N3      | 1:1:2609:A:H2'    | 2.29                     | 0.47              |
| 1:1:1562:G:C5     | 1:1:1563:A:H1'    | 2.49                     | 0.47              |
| 1:1:1682:U:OP1    | 23:5:42:LYS:NZ    | 2.46                     | 0.47              |
| 1:1:1761:U:H2'    | 1:1:1762:G:C4'    | 2.45                     | 0.47              |
| 1:1:2870:G:N7     | 41:AN:49:LYS:HE2  | 2.29                     | 0.47              |
| 1:1:3019:U:O2'    | 1:1:3020:A:H5'    | 2.14                     | 0.47              |
| 1:1:3038:U:H2'    | 1:1:3039:C:C6     | 2.49                     | 0.47              |
| 2:3:3:U:H2'       | 2:3:4:U:H6        | 1.78                     | 0.47              |
| 2:3:31:U:H4'      | 7:m:218:LYS:NZ    | 2.29                     | 0.47              |
| 12:r:179:ASP:OD1  | 12:r:180:GLU:N    | 2.47                     | 0.47              |
| 13:s:13:ARG:HH12  | 13:s:15:GLU:CD    | 2.22                     | 0.47              |
| 14:t:57:VAL:HG22  | 14:t:69:VAL:HG22  | 1.97                     | 0.47              |
| 17:w:28:ILE:HD11  | 17:w:89:ILE:HD11  | 1.97                     | 0.47              |
| 20:z:134:HIS:CE1  | 20:z:136:ARG:HB2  | 2.49                     | 0.47              |
| 28:AA:17:ARG:HA   | 35:AH:73:GLN:O    | 2.15                     | 0.47              |
| 28:AA:103:GLU:HB2 | 28:AA:106:GLN:HB2 | 1.95                     | 0.47              |
| 36:AI:7:PHE:CD1   | 36:AI:8:GLU:HG3   | 2.50                     | 0.47              |
| 46:B:76:A:N6      | 46:B:80:A:O2'     | 2.48                     | 0.47              |
| 46:B:446:C:H2'    | 46:B:447:C:H6     | 1.79                     | 0.47              |
| 46:B:846:U:H5'    | 46:B:847:A:OP2    | 2.13                     | 0.47              |
| 46:B:1783:C:H6    | 73:c:7:SER:HB3    | 1.80                     | 0.47              |
| 51:G:36:HIS:CG    | 51:G:85:GLY:HA3   | 2.50                     | 0.47              |
| 60:P:16:LEU:HG    | 60:P:17:PRO:HD2   | 1.97                     | 0.47              |
| 60:P:136:PRO:HD2  | 60:P:139:TRP:HB2  | 1.96                     | 0.47              |
| 62:R:68:GLU:N     | 62:R:69:PRO:HD3   | 2.30                     | 0.47              |
| 69:Y:40:VAL:HG11  | 69:Y:103:ILE:HD12 | 1.96                     | 0.47              |
| 70:Z:107:PHE:CD2  | 70:Z:114:LYS:HB3  | 2.50                     | 0.47              |
| 1:AS:308:A:H1'    | 1:AS:2200:A:N3    | 2.30                     | 0.47              |
| 1:AS:360:G:N2     | 1:AS:811:G:H1'    | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:513:G:OP1     | 6:AY:347:GLN:NE2   | 2.43                     | 0.47              |
| 1:AS:559:C:H2'     | 1:AS:560:C:C6      | 2.47                     | 0.47              |
| 1:AS:624:U:H2'     | 1:AS:625:C:H6      | 1.80                     | 0.47              |
| 1:AS:1725:A:OP1    | 31:BX:90:GLY:N     | 2.44                     | 0.47              |
| 1:AS:1825:A:H5''   | 1:AS:1826:G:H5'    | 1.96                     | 0.47              |
| 1:AS:2381:G:C8     | 1:AS:2842:C:H4'    | 2.50                     | 0.47              |
| 1:AS:3166:A:C2'    | 1:AS:3167:G:H5'    | 2.44                     | 0.47              |
| 1:AS:3318:G:H3'    | 1:AS:3319:U:O3'    | 2.14                     | 0.47              |
| 5:AX:108:GLU:HG2   | 5:AX:109:HIS:CE1   | 2.49                     | 0.47              |
| 8:BA:20:THR:HG22   | 8:BA:22:LYS:H      | 1.79                     | 0.47              |
| 10:BC:106:LYS:O    | 10:BC:110:LEU:HG   | 2.15                     | 0.47              |
| 11:BD:45:PHE:CE2   | 11:BD:55:ILE:HG12  | 2.50                     | 0.47              |
| 14:BG:88:LYS:O     | 14:BG:92:THR:HG23  | 2.15                     | 0.47              |
| 18:BK:177:ALA:O    | 18:BK:181:ARG:HG3  | 2.14                     | 0.47              |
| 24:BQ:17:LEU:HD13  | 24:BQ:23:MET:HE2   | 1.97                     | 0.47              |
| 25:BR:87:LEU:HD23  | 25:BR:91:LYS:HB2   | 1.96                     | 0.47              |
| 25:BR:99:SER:OG    | 25:BR:102:LYS:NZ   | 2.34                     | 0.47              |
| 26:BS:63:ILE:HG13  | 26:BS:102:LEU:HD12 | 1.96                     | 0.47              |
| 28:BU:83:THR:HG21  | 28:BU:129:TRP:CH2  | 2.50                     | 0.47              |
| 32:BY:54:LEU:HA    | 32:BY:94:PRO:HG3   | 1.97                     | 0.47              |
| 39:CF:61:LYS:O     | 39:CF:65:LEU:HD13  | 2.15                     | 0.47              |
| 42:CI:4:LYS:HB2    | 46:CM:1760:C:OP2   | 2.15                     | 0.47              |
| 45:CL:108:GLY:HA3  | 50:CQ:117:ARG:HG3  | 1.97                     | 0.47              |
| 46:CM:29:U:H2'     | 46:CM:30:G:C8      | 2.48                     | 0.47              |
| 46:CM:237:C:H4'    | 46:CM:238:U:OP1    | 2.14                     | 0.47              |
| 46:CM:324:G:H2'    | 46:CM:325:U:C6     | 2.50                     | 0.47              |
| 46:CM:518:A:H2'    | 46:CM:519:A:H8     | 1.76                     | 0.47              |
| 46:CM:826:U:C5     | 46:CM:827:C:C5     | 3.02                     | 0.47              |
| 46:CM:1129:U:H2'   | 46:CM:1130:U:C6    | 2.49                     | 0.47              |
| 46:CM:1398:G:H4'   | 46:CM:1399:U:O5'   | 2.14                     | 0.47              |
| 46:CM:1593:C:H2'   | 46:CM:1594:G:C8    | 2.49                     | 0.47              |
| 48:CO:171:ILE:HG12 | 48:CO:174:ARG:HH22 | 1.80                     | 0.47              |
| 52:CS:42:LEU:HB3   | 52:CS:46:TRP:CD1   | 2.49                     | 0.47              |
| 52:CS:53:VAL:HG21  | 52:CS:59:VAL:HA    | 1.96                     | 0.47              |
| 52:CS:206:SER:O    | 52:CS:212:LYS:HG2  | 2.14                     | 0.47              |
| 54:CU:30:LEU:HD12  | 54:CU:34:LEU:CD2   | 2.35                     | 0.47              |
| 65:DF:77:THR:HG23  | 65:DF:86:LEU:HD11  | 1.97                     | 0.47              |
| 71:DL:20:ARG:HB3   | 71:DL:76:TYR:CD2   | 2.49                     | 0.47              |
| 79:DT:195:TYR:CZ   | 79:DT:213:LYS:HB2  | 2.50                     | 0.47              |
| 79:DT:291:TRP:CZ3  | 79:DT:298:LEU:HB2  | 2.50                     | 0.47              |
| 81:P0:5:ARG:CA     | 81:P0:8:LYS:HB2    | 2.42                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:P0:22:TYR:HB3  | 81:P0:89:THR:O     | 2.15                     | 0.47              |
| 81:P0:45:LEU:HD21 | 81:P0:99:ILE:O     | 2.14                     | 0.47              |
| 81:P0:77:LEU:O    | 81:P0:79:PHE:N     | 2.40                     | 0.47              |
| 1:1:812:A:N1      | 1:1:915:U:H1'      | 2.30                     | 0.47              |
| 1:1:1022:A:C4     | 1:1:1023:A:H1'     | 2.49                     | 0.47              |
| 1:1:1099:A:N3     | 1:1:1099:A:H2'     | 2.30                     | 0.47              |
| 1:1:1217:A:C2     | 81:P0:12:PHE:CE2   | 2.95                     | 0.47              |
| 1:1:1250:C:H2'    | 1:1:1251:C:C6      | 2.48                     | 0.47              |
| 1:1:1338:G:H2'    | 1:1:1339:A:O4'     | 2.14                     | 0.47              |
| 1:1:1493:C:H2'    | 1:1:1494:A:C8      | 2.49                     | 0.47              |
| 1:1:2980:A:OP2    | 17:w:75:ARG:NH2    | 2.48                     | 0.47              |
| 2:3:96:U:OP1      | 21:0:43:TYR:OH     | 2.30                     | 0.47              |
| 3:4:141:C:O3'     | 16:v:62:TYR:OH     | 2.33                     | 0.47              |
| 13:s:101:ASN:ND2  | 13:s:130:VAL:HG13  | 2.30                     | 0.47              |
| 16:v:73:ARG:HG2   | 16:v:75:VAL:HG13   | 1.97                     | 0.47              |
| 17:w:55:TYR:OH    | 17:w:75:ARG:HD3    | 2.15                     | 0.47              |
| 18:x:126:ARG:HG3  | 18:x:140:GLN:HG2   | 1.95                     | 0.47              |
| 25:7:112:ASP:O    | 25:7:113:LYS:C     | 2.57                     | 0.47              |
| 45:i:93:ARG:HG3   | 45:i:93:ARG:HH11   | 1.79                     | 0.47              |
| 45:i:112:LYS:C    | 45:i:114:GLU:H     | 2.22                     | 0.47              |
| 45:i:116:GLU:O    | 45:i:120:GLU:HG2   | 2.15                     | 0.47              |
| 46:B:503:A:O2'    | 46:B:505:U:OP1     | 2.29                     | 0.47              |
| 46:B:569:G:H5''   | 70:Z:114:LYS:CE    | 2.45                     | 0.47              |
| 46:B:852:G:OP2    | 60:P:3:ARG:NH2     | 2.32                     | 0.47              |
| 46:B:1314:A:OP2   | 50:F:161:SER:OG    | 2.19                     | 0.47              |
| 46:B:1510:G:N7    | 66:V:64:HIS:NE2    | 2.62                     | 0.47              |
| 46:B:1596:U:O2'   | 52:H:105:GLY:O     | 2.18                     | 0.47              |
| 46:B:1628:C:H2'   | 46:B:1629:G:C8     | 2.50                     | 0.47              |
| 48:D:191:GLU:O    | 48:D:195:ARG:HG3   | 2.14                     | 0.47              |
| 53:I:84:TYR:CE1   | 53:I:93:LYS:HB2    | 2.50                     | 0.47              |
| 55:K:67:TRP:NE1   | 55:K:191:GLU:OE2   | 2.48                     | 0.47              |
| 62:R:45:PHE:CD2   | 62:R:49:LEU:HD21   | 2.50                     | 0.47              |
| 79:AR:59:LYS:HD3  | 79:AR:59:LYS:HA    | 1.63                     | 0.47              |
| 79:AR:82:LEU:HD11 | 79:AR:123:ILE:HG12 | 1.97                     | 0.47              |
| 1:AS:284:A:C4     | 1:AS:306:A:H1'     | 2.50                     | 0.47              |
| 1:AS:444:U:O4     | 1:AS:445:A:N6      | 2.48                     | 0.47              |
| 1:AS:1396:U:H2'   | 1:AS:1397:G:O4'    | 2.15                     | 0.47              |
| 1:AS:2515:G:H1'   | 1:AS:2516:U:O4'    | 2.15                     | 0.47              |
| 1:AS:2802:G:H1'   | 1:AS:2833:U:C2     | 2.49                     | 0.47              |
| 8:BA:54:LEU:HD21  | 8:BA:145:LEU:HD11  | 1.97                     | 0.47              |
| 14:BG:170:ARG:O   | 14:BG:174:LEU:HG   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BU:5:ILE:HG22  | 28:BU:28:PRO:HB3   | 1.96                     | 0.47              |
| 45:CL:37:LYS:HD3  | 45:CL:37:LYS:HA    | 1.62                     | 0.47              |
| 45:CL:74:ALA:HB3  | 46:CM:1446:A:H1'   | 1.97                     | 0.47              |
| 45:CL:83:HIS:CE1  | 45:CL:86:LYS:HE3   | 2.49                     | 0.47              |
| 46:CM:399:A:O2'   | 46:CM:400:C:H4'    | 2.15                     | 0.47              |
| 46:CM:515:U:C2    | 46:CM:516:A:C8     | 3.02                     | 0.47              |
| 46:CM:962:A:H2'   | 46:CM:963:A:O4'    | 2.14                     | 0.47              |
| 46:CM:1316:A:OP2  | 46:CM:1317:C:H5    | 1.97                     | 0.47              |
| 46:CM:1375:C:OP2  | 64:DE:45:ARG:HG3   | 2.14                     | 0.47              |
| 46:CM:1772:U:H2'  | 46:CM:1773:G:H8    | 1.79                     | 0.47              |
| 48:CO:32:ILE:HG13 | 48:CO:43:VAL:CG2   | 2.44                     | 0.47              |
| 49:CP:53:LEU:HA   | 68:DI:12:TYR:HE1   | 1.79                     | 0.47              |
| 49:CP:233:SER:OG  | 49:CP:236:GLU:HG2  | 2.15                     | 0.47              |
| 52:CS:26:ALA:HB2  | 63:DD:25:LYS:HB3   | 1.96                     | 0.47              |
| 54:CU:42:ILE:HG23 | 54:CU:55:ALA:O     | 2.15                     | 0.47              |
| 54:CU:68:LYS:C    | 54:CU:72:ARG:HH21  | 2.23                     | 0.47              |
| 79:DT:19:TRP:CE3  | 79:DT:287:ILE:HD13 | 2.50                     | 0.47              |
| 79:DT:273:PRO:HA  | 79:DT:310:TRP:CZ2  | 2.49                     | 0.47              |
| 1:1:236:A:P       | 3:4:95:G:H22       | 2.37                     | 0.47              |
| 1:1:538:G:H2'     | 1:1:539:G:C8       | 2.49                     | 0.47              |
| 1:1:1018:U:H3     | 1:1:1026:A:H61     | 1.62                     | 0.47              |
| 3:4:86:U:H5       | 27:BT:120:GLN:OE1  | 1.97                     | 0.47              |
| 11:q:10:LEU:HD23  | 11:q:11:ASP:N      | 2.30                     | 0.47              |
| 11:q:173:ARG:HE   | 11:q:173:ARG:HB2   | 1.54                     | 0.47              |
| 17:w:2:SER:HB2    | 34:AG:34:GLY:HA2   | 1.97                     | 0.47              |
| 28:AA:40:HIS:CE1  | 28:AA:74:LEU:HD11  | 2.50                     | 0.47              |
| 46:B:432:G:OP1    | 70:Z:78:LYS:HA     | 2.15                     | 0.47              |
| 46:B:744:U:C2     | 46:B:745:A:C8      | 3.03                     | 0.47              |
| 46:B:914:A:OP2    | 46:B:916:C:N4      | 2.45                     | 0.47              |
| 46:B:952:A:OP2    | 60:P:124:ARG:NH2   | 2.40                     | 0.47              |
| 46:B:1369:G:O2'   | 46:B:1370:A:O5'    | 2.25                     | 0.47              |
| 47:C:4:PRO:HD2    | 47:C:7:PHE:CD2     | 2.49                     | 0.47              |
| 53:I:6:SER:O      | 53:I:113:ILE:HG13  | 2.15                     | 0.47              |
| 56:L:92:LYS:C     | 56:L:94:ASP:H      | 2.21                     | 0.47              |
| 59:O:34:THR:HA    | 59:O:37:VAL:HG23   | 1.97                     | 0.47              |
| 59:O:57:ALA:HB1   | 59:O:125:ASN:HB2   | 1.96                     | 0.47              |
| 71:a:39:GLU:OE2   | 71:a:43:LYS:NZ     | 2.47                     | 0.47              |
| 79:AR:130:LYS:HG2 | 79:AR:150:ASP:C    | 2.40                     | 0.47              |
| 1:AS:3179:U:C6    | 8:BA:166:LYS:HE2   | 2.47                     | 0.47              |
| 1:AS:3268:G:H3'   | 1:AS:3342:G:O4'    | 2.14                     | 0.47              |
| 2:AT:85:G:H1'     | 9:BB:218:GLN:NE2   | 2.11                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:AX:209:PHE:CE1  | 5:AX:340:LYS:HG2  | 2.50                     | 0.47              |
| 6:AY:40:PHE:CD2   | 6:AY:243:ALA:HB2  | 2.49                     | 0.47              |
| 10:BC:65:ILE:O    | 10:BC:69:ARG:HG2  | 2.15                     | 0.47              |
| 25:BR:83:VAL:N    | 53:CT:130:PRO:HB2 | 2.30                     | 0.47              |
| 28:BU:89:VAL:HG23 | 28:BU:93:LYS:HG3  | 1.96                     | 0.47              |
| 35:CB:67:LYS:O    | 35:CB:71:THR:HG22 | 2.14                     | 0.47              |
| 42:CI:1:MET:HB2   | 46:CM:1770:C:OP2  | 2.15                     | 0.47              |
| 45:CL:61:GLU:C    | 45:CL:63:ALA:N    | 2.73                     | 0.47              |
| 46:CM:291:U:H2'   | 46:CM:292:C:C6    | 2.50                     | 0.47              |
| 46:CM:819:G:C5    | 46:CM:820:U:C5    | 3.02                     | 0.47              |
| 46:CM:1375:C:O2'  | 64:DE:52:GLY:HA3  | 2.15                     | 0.47              |
| 48:CO:58:ALA:O    | 48:CO:62:LYS:N    | 2.39                     | 0.47              |
| 52:CS:21:GLN:CD   | 52:CS:22:VAL:H    | 2.23                     | 0.47              |
| 52:CS:80:LYS:HG3  | 52:CS:83:ARG:NH2  | 2.30                     | 0.47              |
| 53:CT:1:MET:HE2   | 53:CT:106:LEU:HB2 | 1.96                     | 0.47              |
| 59:CZ:57:ALA:HA   | 59:CZ:123:VAL:O   | 2.14                     | 0.47              |
| 81:P0:66:PHE:HE2  | 81:P0:70:LEU:HD12 | 1.79                     | 0.47              |
| 1:1:385:A:H2'     | 1:1:386:A:C8      | 2.50                     | 0.47              |
| 1:1:514:G:H2'     | 1:1:516:U:H5'     | 1.97                     | 0.47              |
| 1:1:1012:U:C4'    | 1:1:1013:U:H4'    | 2.45                     | 0.47              |
| 1:1:2220:A:H5''   | 4:j:244:GLY:HA3   | 1.96                     | 0.47              |
| 1:1:2447:G:O2'    | 1:1:2448:C:O5'    | 2.32                     | 0.47              |
| 5:k:71:GLU:OE2    | 5:k:357:LYS:NZ    | 2.48                     | 0.47              |
| 6:l:30:PRO:HB3    | 19:y:25:TYR:HE2   | 1.80                     | 0.47              |
| 45:i:114:GLU:HG2  | 45:i:115:LEU:H    | 1.79                     | 0.47              |
| 46:B:68:A:OP1     | 53:I:160:ARG:NH2  | 2.41                     | 0.47              |
| 46:B:611:G:OP2    | 46:B:1084:U:O2'   | 2.23                     | 0.47              |
| 46:B:938:G:H2'    | 46:B:939:G:C8     | 2.50                     | 0.47              |
| 46:B:1642:A:N6    | 46:B:1732:G:O2'   | 2.48                     | 0.47              |
| 65:U:123:ARG:HG3  | 65:U:133:VAL:HB   | 1.97                     | 0.47              |
| 78:h:175:ALA:O    | 78:h:177:MET:HG3  | 2.15                     | 0.47              |
| 1:AS:350:C:HO2'   | 1:AS:367:A:H2     | 1.60                     | 0.47              |
| 1:AS:1079:G:H2'   | 1:AS:1080:A:H8    | 1.80                     | 0.47              |
| 1:AS:1140:U:OP1   | 1:AS:1363:G:O2'   | 2.30                     | 0.47              |
| 1:AS:1151:C:H2'   | 1:AS:1152:C:C6    | 2.50                     | 0.47              |
| 1:AS:2183:U:O4    | 1:AS:2216:G:N1    | 2.48                     | 0.47              |
| 7:AZ:269:SER:O    | 7:AZ:273:ARG:HG2  | 2.15                     | 0.47              |
| 80:BE:63:GLU:OE1  | 80:BE:63:GLU:N    | 2.44                     | 0.47              |
| 14:BG:196:GLU:HA  | 14:BG:199:LYS:HB3 | 1.97                     | 0.47              |
| 35:CB:108:GLN:HA  | 35:CB:111:LYS:NZ  | 2.29                     | 0.47              |
| 46:CM:17:C:H2'    | 46:CM:18:C:H6     | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:119:A:H1'    | 46:CM:395:A:C4     | 2.50                     | 0.47              |
| 46:CM:136:U:HO2'   | 53:CT:149:LYS:HZ2  | 1.51                     | 0.47              |
| 46:CM:379:C:H5''   | 51:CR:10:LYS:HD3   | 1.97                     | 0.47              |
| 46:CM:823:G:H2'    | 46:CM:824:U:C5     | 2.49                     | 0.47              |
| 46:CM:1436:U:H2'   | 46:CM:1437:C:C6    | 2.50                     | 0.47              |
| 46:CM:1485:G:H2'   | 46:CM:1486:G:H8    | 1.80                     | 0.47              |
| 46:CM:1551:U:H2'   | 46:CM:1552:C:C6    | 2.50                     | 0.47              |
| 48:CO:127:VAL:HG13 | 48:CO:176:VAL:HG11 | 1.96                     | 0.47              |
| 55:CV:190:LEU:HD22 | 55:CV:194:GLU:HG2  | 1.96                     | 0.47              |
| 75:DP:12:VAL:CG2   | 75:DP:52:ASP:H     | 2.26                     | 0.47              |
| 79:DT:158:SER:C    | 79:DT:160:SER:N    | 2.71                     | 0.47              |
| 82:12:104:ILE:HD11 | 82:12:142:ARG:CB   | 2.36                     | 0.47              |
| 1:1:208:A:H4'      | 1:1:210:A:C8       | 2.50                     | 0.46              |
| 1:1:653:C:H5''     | 33:AF:27:HIS:HB3   | 1.96                     | 0.46              |
| 1:1:1069:U:H2'     | 1:1:1070:U:C6      | 2.50                     | 0.46              |
| 1:1:1627:C:H5''    | 1:1:1628:A:H5''    | 1.97                     | 0.46              |
| 1:1:3021:A:C5      | 5:k:75:ALA:HB2     | 2.51                     | 0.46              |
| 5:k:229:VAL:HG21   | 5:k:249:VAL:HG23   | 1.97                     | 0.46              |
| 31:AD:19:THR:HG23  | 31:AD:97:ALA:HA    | 1.97                     | 0.46              |
| 33:AF:97:ILE:HG21  | 33:AF:106:ARG:HG3  | 1.97                     | 0.46              |
| 46:B:12:U:H2'      | 46:B:13:C:H6       | 1.78                     | 0.46              |
| 46:B:66:U:O4       | 53:I:134:GLY:N     | 2.38                     | 0.46              |
| 46:B:345:G:H5''    | 58:N:80:MET:HE2    | 1.96                     | 0.46              |
| 46:B:638:U:H2'     | 46:B:639:G:O4'     | 2.15                     | 0.46              |
| 46:B:1110:A:C5     | 46:B:1111:G:H1'    | 2.51                     | 0.46              |
| 46:B:1161:G:C6     | 46:B:1450:G:C6     | 3.03                     | 0.46              |
| 46:B:1484:U:C4     | 46:B:1498:G:C2     | 3.03                     | 0.46              |
| 50:F:151:GLN:OE1   | 50:F:153:TYR:OH    | 2.07                     | 0.46              |
| 52:H:140:SER:OG    | 52:H:171:ALA:HB1   | 2.15                     | 0.46              |
| 52:H:149:ILE:O     | 52:H:156:ARG:NH2   | 2.48                     | 0.46              |
| 54:J:135:ARG:O     | 54:J:147:LYS:N     | 2.41                     | 0.46              |
| 1:AS:1313:A:O2'    | 1:AS:1314:A:H3'    | 2.15                     | 0.46              |
| 1:AS:1493:C:H2'    | 1:AS:1494:A:H8     | 1.79                     | 0.46              |
| 1:AS:2777:G:N3     | 1:AS:2939:A:H2     | 2.14                     | 0.46              |
| 20:BM:165:ARG:HH21 | 46:CM:799:G:H5''   | 1.80                     | 0.46              |
| 23:BP:80:LYS:O     | 23:BP:84:LYS:HB2   | 2.15                     | 0.46              |
| 26:BS:67:ILE:HD12  | 26:BS:83:VAL:HG12  | 1.96                     | 0.46              |
| 28:BU:84:ARG:NH1   | 35:CB:97:GLU:OE1   | 2.48                     | 0.46              |
| 28:BU:99:GLU:OE1   | 28:BU:99:GLU:N     | 2.47                     | 0.46              |
| 46:CM:211:A:H3'    | 46:CM:212:G:H8     | 1.80                     | 0.46              |
| 46:CM:598:U:P      | 70:DK:108:GLY:HA2  | 2.55                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:CM:721:C:H42   | 46:CM:722:A:N6    | 2.14                     | 0.46              |
| 46:CM:992:C:OP1   | 61:DB:130:ARG:HA  | 2.15                     | 0.46              |
| 46:CM:1211:A:O2'  | 46:CM:1241:A:N1   | 2.35                     | 0.46              |
| 46:CM:1243:U:C6   | 46:CM:1244:U:H5   | 2.33                     | 0.46              |
| 46:CM:1253:G:H1'  | 46:CM:1434:G:H4'  | 1.97                     | 0.46              |
| 46:CM:1668:A:H2'  | 46:CM:1669:U:H5'  | 1.97                     | 0.46              |
| 48:CO:180:THR:OG1 | 48:CO:183:GLN:HG3 | 2.14                     | 0.46              |
| 49:CP:96:VAL:HG21 | 49:CP:203:GLU:HG3 | 1.96                     | 0.46              |
| 49:CP:171:LYS:HE2 | 56:CW:57:ARG:NH1  | 2.30                     | 0.46              |
| 54:CU:37:LEU:HD22 | 54:CU:66:TYR:CE2  | 2.50                     | 0.46              |
| 79:DT:164:SER:OG  | 79:DT:180:LEU:N   | 2.48                     | 0.46              |
| 79:DT:204:ASP:OD1 | 79:DT:204:ASP:N   | 2.47                     | 0.46              |
| 1:1:663:A:OP1     | 16:v:203:ARG:HD2  | 2.15                     | 0.46              |
| 1:1:663:A:H1'     | 14:t:14:PHE:CZ    | 2.51                     | 0.46              |
| 1:1:677:U:H2'     | 1:1:678:G:C8      | 2.50                     | 0.46              |
| 1:1:1725:A:C6     | 44:AQ:42:CYS:HA   | 2.50                     | 0.46              |
| 2:3:7:G:O3'       | 7:m:33:ARG:NH2    | 2.48                     | 0.46              |
| 2:3:11:A:N6       | 7:m:16:PHE:O      | 2.48                     | 0.46              |
| 14:t:133:SER:HA   | 14:BG:129:LYS:CE  | 2.44                     | 0.46              |
| 35:AH:67:LYS:O    | 35:AH:71:THR:HG22 | 2.15                     | 0.46              |
| 37:AJ:69:LYS:HD3  | 37:AJ:79:HIS:NE2  | 2.30                     | 0.46              |
| 38:AK:36:SER:OG   | 38:AK:57:ARG:NH2  | 2.48                     | 0.46              |
| 46:B:55:A:OP1     | 71:a:112:LYS:NZ   | 2.35                     | 0.46              |
| 46:B:236:U:O2'    | 46:B:237:C:H3'    | 2.15                     | 0.46              |
| 46:B:740:A:O2'    | 46:B:741:A:OP1    | 2.30                     | 0.46              |
| 46:B:1072:A:H2'   | 46:B:1073:A:C8    | 2.50                     | 0.46              |
| 56:L:65:LYS:HA    | 56:L:70:LEU:HD11  | 1.96                     | 0.46              |
| 61:Q:81:THR:HG21  | 61:Q:85:LYS:HD2   | 1.97                     | 0.46              |
| 66:V:109:GLN:HG3  | 66:V:114:LEU:CD1  | 2.45                     | 0.46              |
| 79:AR:113:SER:OG  | 79:AR:155:VAL:N   | 2.48                     | 0.46              |
| 1:AS:7:C:H42      | 3:AU:150:G:H1     | 1.63                     | 0.46              |
| 1:AS:25:A:H5'     | 1:AS:329:U:H2'    | 1.96                     | 0.46              |
| 1:AS:666:G:H5'    | 14:BG:8:PRO:HG2   | 1.97                     | 0.46              |
| 1:AS:1020:G:H4'   | 1:AS:1020:G:OP1   | 2.14                     | 0.46              |
| 1:AS:2326:A:O2'   | 1:AS:2369:G:OP1   | 2.22                     | 0.46              |
| 1:AS:2584:U:H2'   | 1:AS:2585:U:O4'   | 2.15                     | 0.46              |
| 1:AS:2729:U:H4'   | 22:BO:7:TYR:HB3   | 1.97                     | 0.46              |
| 1:AS:2985:U:H2'   | 1:AS:2986:U:C6    | 2.50                     | 0.46              |
| 1:AS:3081:G:N2    | 11:BD:156:GLN:OE1 | 2.48                     | 0.46              |
| 1:AS:3150:A:C4    | 17:BJ:115:LYS:HA  | 2.51                     | 0.46              |
| 2:AT:90:A:H2'     | 2:AT:91:G:O4'     | 2.14                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AU:90:U:H1'     | 27:BT:25:VAL:HG23  | 1.97                     | 0.46              |
| 14:BG:76:THR:HG22 | 14:BG:101:ARG:HB3  | 1.96                     | 0.46              |
| 18:BK:19:GLY:HA3  | 18:BK:22:LEU:HD11  | 1.96                     | 0.46              |
| 23:BP:99:VAL:HG21 | 23:BP:109:GLN:NE2  | 2.29                     | 0.46              |
| 35:CB:108:GLN:HA  | 35:CB:108:GLN:OE1  | 2.16                     | 0.46              |
| 37:CD:57:ILE:HD13 | 37:CD:89:MET:HB3   | 1.96                     | 0.46              |
| 45:CL:116:GLU:O   | 45:CL:120:GLU:HB2  | 2.16                     | 0.46              |
| 46:CM:25:C:H4'    | 46:CM:26:A:O5'     | 2.14                     | 0.46              |
| 46:CM:289:G:H2'   | 46:CM:290:U:C6     | 2.50                     | 0.46              |
| 46:CM:510:A:H4'   | 56:CW:164:TYR:HE1  | 1.79                     | 0.46              |
| 46:CM:826:U:C5    | 46:CM:827:C:H5     | 2.33                     | 0.46              |
| 46:CM:845:U:O4'   | 54:CU:110:ARG:HG3  | 2.15                     | 0.46              |
| 46:CM:1396:A:HO2' | 46:CM:1397:A:P     | 2.38                     | 0.46              |
| 50:CQ:105:ALA:O   | 50:CQ:109:LYS:HG2  | 2.15                     | 0.46              |
| 54:CU:66:TYR:O    | 54:CU:70:GLN:HB2   | 2.15                     | 0.46              |
| 58:CY:36:LYS:HE2  | 58:CY:36:LYS:HB3   | 1.80                     | 0.46              |
| 62:DC:44:ARG:HD2  | 62:DC:44:ARG:HA    | 1.68                     | 0.46              |
| 65:DF:72:ILE:HD13 | 65:DF:79:TYR:CD2   | 2.51                     | 0.46              |
| 69:DJ:8:ALA:HB2   | 69:DJ:74:VAL:HG21  | 1.97                     | 0.46              |
| 78:DS:174:MET:SD  | 78:DS:188:LEU:HD21 | 2.56                     | 0.46              |
| 79:DT:134:VAL:O   | 79:DT:141:CYS:HA   | 2.15                     | 0.46              |
| 79:DT:251:ALA:O   | 79:DT:257:ILE:HA   | 2.15                     | 0.46              |
| 1:1:216:U:H4'     | 27:9:100:HIS:CG    | 2.50                     | 0.46              |
| 1:1:532:U:H2'     | 1:1:533:G:C8       | 2.51                     | 0.46              |
| 1:1:623:A:H2'     | 1:1:624:U:H6       | 1.78                     | 0.46              |
| 1:1:845:C:H2'     | 1:1:846:U:H6       | 1.80                     | 0.46              |
| 1:1:925:A:H2'     | 1:1:926:U:C6       | 2.50                     | 0.46              |
| 1:1:1140:U:OP2    | 33:AF:44:ARG:NH1   | 2.47                     | 0.46              |
| 1:1:2621:G:H4'    | 1:1:2668:A:O4'     | 2.15                     | 0.46              |
| 2:3:59:U:H2'      | 2:3:60:G:C8        | 2.51                     | 0.46              |
| 6:l:54:ALA:HB3    | 6:l:57:ALA:HB2     | 1.96                     | 0.46              |
| 9:o:75:VAL:HG11   | 21:0:57:GLU:OE2    | 2.15                     | 0.46              |
| 10:p:114:ALA:HA   | 10:p:117:ILE:HG22  | 1.97                     | 0.46              |
| 14:t:2:ALA:HB1    | 29:AB:33:GLY:O     | 2.15                     | 0.46              |
| 46:B:1706:A:H2'   | 46:B:1707:G:O4'    | 2.15                     | 0.46              |
| 51:G:105:VAL:HG21 | 51:G:245:ILE:C     | 2.39                     | 0.46              |
| 61:Q:20:ASP:N     | 61:Q:50:SER:HB3    | 2.30                     | 0.46              |
| 1:AS:134:U:C2     | 36:CC:94:LYS:HG3   | 2.50                     | 0.46              |
| 1:AS:212:A:N6     | 1:AS:226:G:O2'     | 2.48                     | 0.46              |
| 1:AS:560:C:H2'    | 1:AS:561:U:C6      | 2.50                     | 0.46              |
| 1:AS:1921:U:H1'   | 44:CK:20:SER:HB3   | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:2978:A:H2'    | 1:AS:2979:U:O4'    | 2.15                     | 0.46              |
| 10:BC:201:LEU:HD23 | 10:BC:201:LEU:HA   | 1.79                     | 0.46              |
| 14:BG:21:ARG:NH1   | 16:BI:191:TRP:HH2  | 2.13                     | 0.46              |
| 14:BG:64:LYS:HD2   | 29:BV:69:TRP:CD1   | 2.50                     | 0.46              |
| 19:BL:96:PHE:CD1   | 19:BL:97:PRO:HD2   | 2.51                     | 0.46              |
| 28:BU:3:LYS:HE2    | 28:BU:5:ILE:O      | 2.15                     | 0.46              |
| 29:BV:28:HIS:CD2   | 29:BV:32:ARG:HG2   | 2.49                     | 0.46              |
| 46:CM:66:U:H4'     | 53:CT:171:LYS:HB3  | 1.98                     | 0.46              |
| 46:CM:246:U:H5'    | 58:CY:36:LYS:HG3   | 1.97                     | 0.46              |
| 46:CM:291:U:H2'    | 46:CM:292:C:H6     | 1.80                     | 0.46              |
| 46:CM:474:U:C2     | 77:DR:31:GLN:HG3   | 2.51                     | 0.46              |
| 46:CM:474:U:H2'    | 77:DR:31:GLN:HE21  | 1.81                     | 0.46              |
| 47:CN:63:ILE:HD11  | 47:CN:158:VAL:HG21 | 1.96                     | 0.46              |
| 48:CO:29:TRP:HZ2   | 61:DB:69:VAL:HG12  | 1.78                     | 0.46              |
| 48:CO:149:GLN:HE21 | 48:CO:151:LYS:HG3  | 1.79                     | 0.46              |
| 50:CQ:179:ARG:H    | 50:CQ:179:ARG:HD2  | 1.79                     | 0.46              |
| 54:CU:30:LEU:CD1   | 54:CU:34:LEU:HD21  | 2.38                     | 0.46              |
| 59:CZ:42:ALA:CB    | 59:CZ:122:VAL:HB   | 2.46                     | 0.46              |
| 59:CZ:82:PRO:HB2   | 59:CZ:83:GLU:H     | 1.48                     | 0.46              |
| 65:DF:57:ARG:NH1   | 72:DM:40:VAL:HB    | 2.31                     | 0.46              |
| 69:DJ:115:GLU:O    | 69:DJ:119:LYS:HG2  | 2.15                     | 0.46              |
| 1:1:597:U:H2'      | 1:1:598:U:H4'      | 1.95                     | 0.46              |
| 1:1:1312:C:H5'     | 1:1:1313:A:C2      | 2.49                     | 0.46              |
| 1:1:2988:A:H2'     | 1:1:2989:A:C8      | 2.49                     | 0.46              |
| 7:m:160:PHE:O      | 7:m:163:LEU:HB3    | 2.15                     | 0.46              |
| 8:n:39:LEU:HD13    | 8:n:83:VAL:HG11    | 1.97                     | 0.46              |
| 32:AE:9:ARG:HG2    | 32:AE:107:VAL:HA   | 1.97                     | 0.46              |
| 35:AH:54:ILE:HD11  | 35:AH:78:GLY:HA2   | 1.96                     | 0.46              |
| 37:AJ:60:ILE:HG21  | 37:AJ:90:THR:HG22  | 1.96                     | 0.46              |
| 45:i:47:ASP:C      | 45:i:49:ALA:N      | 2.73                     | 0.46              |
| 46:B:348:U:OP1     | 58:N:104:HIS:HE1   | 1.99                     | 0.46              |
| 46:B:814:A:HO2'    | 46:B:815:U:P       | 2.37                     | 0.46              |
| 46:B:869:A:N6      | 46:B:913:U:H3      | 2.13                     | 0.46              |
| 47:C:6:SER:O       | 47:C:191:ARG:NH1   | 2.49                     | 0.46              |
| 54:J:33:GLU:HG2    | 54:J:34:LEU:HD12   | 1.96                     | 0.46              |
| 56:L:10:LYS:HE3    | 56:L:12:TYR:O      | 2.16                     | 0.46              |
| 62:R:80:LEU:HD12   | 62:R:83:MET:HB2    | 1.97                     | 0.46              |
| 1:AS:624:U:H2'     | 1:AS:625:C:C6      | 2.49                     | 0.46              |
| 1:AS:1444:U:H5''   | 18:BK:66:SER:O     | 2.16                     | 0.46              |
| 1:AS:1707:U:C4     | 1:AS:1708:G:C6     | 3.03                     | 0.46              |
| 1:AS:2639:A:H2'    | 1:AS:2640:U:O4'    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:BC:246:LYS:O   | 10:BC:250:LYS:HG3  | 2.16                     | 0.46              |
| 23:BP:36:TYR:HE1  | 23:BP:82:LEU:HD22  | 1.79                     | 0.46              |
| 28:BU:83:THR:HG21 | 28:BU:129:TRP:HH2  | 1.81                     | 0.46              |
| 36:CC:29:ALA:O    | 36:CC:33:VAL:HG23  | 2.15                     | 0.46              |
| 46:CM:257:U:OP1   | 55:CV:75:LYS:NZ    | 2.32                     | 0.46              |
| 46:CM:449:G:H2'   | 46:CM:451:C:C5     | 2.51                     | 0.46              |
| 46:CM:811:U:H2'   | 46:CM:812:C:C6     | 2.50                     | 0.46              |
| 46:CM:1110:A:C5   | 46:CM:1111:G:H1'   | 2.50                     | 0.46              |
| 46:CM:1312:C:C2   | 46:CM:1313:G:C8    | 3.03                     | 0.46              |
| 46:CM:1376:U:H5'' | 64:DE:3:ARG:HD2    | 1.96                     | 0.46              |
| 46:CM:1512:A:H4'  | 66:DG:83:ALA:HB2   | 1.97                     | 0.46              |
| 52:CS:28:THR:C    | 52:CS:29:ILE:HD13  | 2.40                     | 0.46              |
| 52:CS:29:ILE:HG22 | 52:CS:33:VAL:HG13  | 1.97                     | 0.46              |
| 54:CU:56:VAL:HG12 | 54:CU:58:VAL:HG23  | 1.97                     | 0.46              |
| 75:DP:65:ARG:N    | 75:DP:65:ARG:HD2   | 2.31                     | 0.46              |
| 79:DT:13:LEU:HB3  | 79:DT:45:TRP:CZ2   | 2.50                     | 0.46              |
| 79:DT:133:LYS:HB3 | 79:DT:135:TRP:HE1  | 1.81                     | 0.46              |
| 79:DT:172:ASP:OD2 | 79:DT:174:THR:OG1  | 2.32                     | 0.46              |
| 1:1:240:C:H5'     | 1:1:241:C:H5''     | 1.98                     | 0.46              |
| 1:1:798:C:H2'     | 1:1:799:C:H6       | 1.79                     | 0.46              |
| 1:1:1148:G:OP2    | 1:1:1148:G:N2      | 2.48                     | 0.46              |
| 1:1:1252:G:H2'    | 1:1:1253:C:C6      | 2.50                     | 0.46              |
| 1:1:2367:C:H2'    | 1:1:2368:A:C8      | 2.50                     | 0.46              |
| 1:1:2404:U:H2'    | 1:1:2405:U:H6      | 1.81                     | 0.46              |
| 1:1:3016:A:H2'    | 1:1:3017:G:C8      | 2.50                     | 0.46              |
| 1:1:3039:C:H3'    | 20:z:62:ARG:HH22   | 1.80                     | 0.46              |
| 1:1:3067:U:H2'    | 1:1:3068:C:H6      | 1.81                     | 0.46              |
| 7:m:178:ASN:HA    | 7:m:183:TRP:CD2    | 2.51                     | 0.46              |
| 12:r:140:THR:HG21 | 12:r:148:VAL:HG21  | 1.97                     | 0.46              |
| 22:2:112:ASN:HB3  | 22:2:128:LEU:HD13  | 1.98                     | 0.46              |
| 25:7:113:LYS:HD2  | 25:7:113:LYS:HA    | 1.68                     | 0.46              |
| 32:AE:43:MET:HE3  | 32:AE:76:ARG:HB2   | 1.97                     | 0.46              |
| 32:AE:71:ARG:HH11 | 32:AE:103:LEU:HD13 | 1.80                     | 0.46              |
| 39:AL:3:ARG:O     | 39:AL:52:TYR:HA    | 2.15                     | 0.46              |
| 46:B:1149:G:H2'   | 46:B:1150:G:C8     | 2.51                     | 0.46              |
| 46:B:1364:U:O2'   | 46:B:1365:C:H5'    | 2.16                     | 0.46              |
| 46:B:1396:A:HO2'  | 46:B:1397:A:P      | 2.38                     | 0.46              |
| 46:B:1742:A:OP1   | 70:Z:63:GLN:HG2    | 2.16                     | 0.46              |
| 49:E:53:LEU:O     | 68:X:15:ARG:NE     | 2.49                     | 0.46              |
| 57:M:14:TYR:CD2   | 57:M:21:VAL:HG22   | 2.49                     | 0.46              |
| 73:c:26:CYS:HB3   | 73:c:77:CYS:SG     | 2.55                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AS:122:A:C6     | 1:AS:149:A:C5     | 3.03                     | 0.46              |
| 1:AS:1493:C:H2'   | 1:AS:1494:A:C8    | 2.51                     | 0.46              |
| 1:AS:2538:A:N1    | 10:BC:33:LYS:HB2  | 2.31                     | 0.46              |
| 1:AS:3172:U:O4    | 21:BN:159:SER:HB2 | 2.15                     | 0.46              |
| 5:AX:47:LEU:HB2   | 5:AX:84:MET:SD    | 2.55                     | 0.46              |
| 28:BU:10:VAL:O    | 28:BU:83:THR:OG1  | 2.33                     | 0.46              |
| 37:CD:59:LEU:HD11 | 37:CD:67:ARG:HD3  | 1.97                     | 0.46              |
| 46:CM:215:A:N3    | 46:CM:215:A:H2'   | 2.31                     | 0.46              |
| 46:CM:238:U:O2'   | 46:CM:239:U:OP1   | 2.34                     | 0.46              |
| 46:CM:695:C:HO2'  | 46:CM:696:U:P     | 2.34                     | 0.46              |
| 46:CM:1086:G:H4'  | 69:DJ:76:GLN:HG3  | 1.98                     | 0.46              |
| 48:CO:138:PHE:HB3 | 48:CO:213:ARG:NE  | 2.30                     | 0.46              |
| 51:CR:112:HIS:NE2 | 51:CR:238:SER:O   | 2.46                     | 0.46              |
| 52:CS:64:ILE:HG13 | 52:CS:65:ARG:N    | 2.31                     | 0.46              |
| 62:DC:1:MET:HE2   | 65:DF:19:ASN:N    | 2.31                     | 0.46              |
| 62:DC:90:ILE:O    | 62:DC:90:ILE:HG22 | 2.16                     | 0.46              |
| 70:DK:29:TYR:HA   | 70:DK:32:ARG:HH12 | 1.80                     | 0.46              |
| 1:1:256:G:H4'     | 36:AI:111:PHE:HZ  | 1.80                     | 0.46              |
| 1:1:269:G:H5'     | 16:v:120:TRP:CE3  | 2.50                     | 0.46              |
| 1:1:795:G:O2'     | 14:t:18:TRP:NE1   | 2.38                     | 0.46              |
| 1:1:1020:G:H2'    | 1:1:1022:A:N7     | 2.31                     | 0.46              |
| 1:1:1237:U:H2'    | 1:1:1239:G:OP2    | 2.16                     | 0.46              |
| 1:1:1278:G:H4'    | 81:P0:83:ASN:N    | 2.31                     | 0.46              |
| 1:1:2681:C:H2'    | 1:1:2682:C:C6     | 2.49                     | 0.46              |
| 1:1:2946:U:H2'    | 1:1:2947:U:C6     | 2.51                     | 0.46              |
| 7:m:150:LEU:HD12  | 13:s:143:ARG:HG3  | 1.97                     | 0.46              |
| 9:o:13:LYS:HA     | 9:o:13:LYS:HE2    | 1.97                     | 0.46              |
| 23:5:30:GLN:HE21  | 23:5:58:ALA:HB1   | 1.80                     | 0.46              |
| 46:B:561:U:C5     | 46:B:578:A:N7     | 2.84                     | 0.46              |
| 46:B:673:A:H2'    | 46:B:674:C:O4'    | 2.16                     | 0.46              |
| 46:B:741:A:H5'    | 51:G:16:SER:OG    | 2.15                     | 0.46              |
| 46:B:992:C:OP1    | 61:Q:130:ARG:HA   | 2.16                     | 0.46              |
| 46:B:1393:U:H2'   | 46:B:1394:G:C8    | 2.50                     | 0.46              |
| 46:B:1414:G:H3'   | 46:B:1414:G:OP2   | 2.16                     | 0.46              |
| 46:B:1602:C:P     | 52:H:81:ARG:HE    | 2.37                     | 0.46              |
| 46:B:1774:C:H2'   | 46:B:1775:G:C8    | 2.50                     | 0.46              |
| 58:N:26:LYS:HZ2   | 58:N:29:LYS:HD2   | 1.80                     | 0.46              |
| 61:Q:65:LYS:O     | 61:Q:69:VAL:HG23  | 2.15                     | 0.46              |
| 69:Y:3:ARG:NH1    | 69:Y:9:ASP:OD2    | 2.49                     | 0.46              |
| 69:Y:24:GLN:HA    | 69:Y:63:VAL:O     | 2.16                     | 0.46              |
| 1:AS:582:G:H2'    | 1:AS:583:A:C8     | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:726:G:H5'     | 19:BL:47:VAL:HG21  | 1.98                     | 0.46              |
| 1:AS:730:A:C8      | 1:AS:734:G:C6      | 3.03                     | 0.46              |
| 1:AS:948:A:C2      | 1:AS:1110:U:H4'    | 2.50                     | 0.46              |
| 1:AS:2196:G:H2'    | 1:AS:2197:A:H8     | 1.80                     | 0.46              |
| 1:AS:2502:A:H2     | 10:BC:45:ARG:HE    | 1.63                     | 0.46              |
| 1:AS:3316:U:O2'    | 1:AS:3317:U:OP1    | 2.32                     | 0.46              |
| 1:AS:3339:U:H2'    | 1:AS:3343:C:H41    | 1.81                     | 0.46              |
| 6:AY:11:SER:OG     | 6:AY:15:GLU:OE1    | 2.34                     | 0.46              |
| 10:BC:141:VAL:O    | 10:BC:145:GLU:HG3  | 2.15                     | 0.46              |
| 16:BI:28:TRP:CD2   | 16:BI:28:TRP:C     | 2.94                     | 0.46              |
| 20:BM:154:ALA:O    | 20:BM:158:GLU:CD   | 2.59                     | 0.46              |
| 37:CD:86:VAL:O     | 37:CD:87:GLU:C     | 2.58                     | 0.46              |
| 46:CM:147:C:OP1    | 71:DL:121:THR:OG1  | 2.20                     | 0.46              |
| 46:CM:222:C:H2'    | 46:CM:223:A:O4'    | 2.16                     | 0.46              |
| 46:CM:726:C:O2     | 54:CU:103:ARG:NH2  | 2.49                     | 0.46              |
| 46:CM:1192:C:N3    | 46:CM:1442:C:H5    | 2.14                     | 0.46              |
| 46:CM:1211:A:H61   | 59:CZ:114:LYS:HD3  | 1.81                     | 0.46              |
| 46:CM:1218:G:N1    | 46:CM:1238:U:O2    | 2.48                     | 0.46              |
| 46:CM:1226:G:C4    | 62:DC:79:HIS:CD2   | 3.03                     | 0.46              |
| 46:CM:1258:G:N7    | 46:CM:1416:U:H3'   | 2.31                     | 0.46              |
| 47:CN:15:LYS:NZ    | 64:DE:93:LEU:HD13  | 2.31                     | 0.46              |
| 49:CP:78:ILE:HD11  | 49:CP:120:ILE:HD11 | 1.96                     | 0.46              |
| 51:CR:59:ARG:HH22  | 71:DL:87:PRO:HG3   | 1.80                     | 0.46              |
| 52:CS:102:ARG:C    | 52:CS:103:ASN:HD22 | 2.24                     | 0.46              |
| 59:CZ:43:ARG:H     | 59:CZ:43:ARG:HG2   | 1.54                     | 0.46              |
| 59:CZ:76:GLU:O     | 59:CZ:80:ASN:CG    | 2.58                     | 0.46              |
| 69:DJ:106:THR:HG22 | 69:DJ:109:GLY:O    | 2.15                     | 0.46              |
| 81:P0:73:PHE:HA    | 81:P0:76:LEU:HG    | 1.98                     | 0.46              |
| 82:12:114:ARG:HH21 | 82:12:125:LEU:CD1  | 2.27                     | 0.46              |
| 1:1:431:A:H2'      | 1:1:432:G:H8       | 1.80                     | 0.46              |
| 1:1:1233:G:H1      | 1:1:1247:A:N6      | 2.01                     | 0.46              |
| 1:1:2293:G:C2      | 1:1:2294:G:N7      | 2.84                     | 0.46              |
| 1:1:2376:A:OP1     | 1:1:2845:U:H4'     | 2.16                     | 0.46              |
| 1:1:2995:U:H2'     | 1:1:2996:A:H8      | 1.81                     | 0.46              |
| 1:1:2999:A:H2'     | 1:1:3000:G:O4'     | 2.16                     | 0.46              |
| 1:1:3135:A:H2'     | 1:1:3136:C:C6      | 2.50                     | 0.46              |
| 6:l:149:LEU:HA     | 6:l:150:PRO:C      | 2.39                     | 0.46              |
| 12:r:4:ARG:CZ      | 12:r:99:ILE:HG13   | 2.45                     | 0.46              |
| 13:s:46:VAL:HG23   | 13:s:68:HIS:CD2    | 2.50                     | 0.46              |
| 20:z:173:ARG:O     | 20:z:177:LEU:HG    | 2.15                     | 0.46              |
| 38:AK:27:PHE:HA    | 38:AK:34:CYS:HA    | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:473:A:OP1    | 56:L:126:ARG:HD3   | 2.16                     | 0.46              |
| 46:B:671:G:C3'    | 46:B:672:U:H5'     | 2.36                     | 0.46              |
| 46:B:823:G:H2'    | 46:B:824:U:C4      | 2.50                     | 0.46              |
| 46:B:1155:G:C2    | 46:B:1156:A:C8     | 3.02                     | 0.46              |
| 46:B:1317:C:O2'   | 50:F:163:GLN:HB3   | 2.16                     | 0.46              |
| 46:B:1669:U:O2'   | 46:B:1670:U:H6     | 1.97                     | 0.46              |
| 52:H:89:ILE:HD11  | 52:H:172:ILE:HD11  | 1.98                     | 0.46              |
| 74:d:36:LYS:O     | 74:d:77:CYS:HA     | 2.16                     | 0.46              |
| 79:AR:135:TRP:CZ3 | 79:AR:141:CYS:HB2  | 2.51                     | 0.46              |
| 1:AS:209:C:C2     | 1:AS:229:C:H4'     | 2.51                     | 0.46              |
| 1:AS:259:C:H2'    | 1:AS:260:C:H6      | 1.81                     | 0.46              |
| 1:AS:413:U:H2'    | 1:AS:414:U:H6      | 1.81                     | 0.46              |
| 1:AS:2826:U:OP1   | 80:BE:61:SER:OG    | 2.34                     | 0.46              |
| 1:AS:2972:A:H2'   | 1:AS:2973:U:C6     | 2.51                     | 0.46              |
| 1:AS:2978:A:C2    | 1:AS:3113:A:C4     | 3.03                     | 0.46              |
| 1:AS:3111:A:O4'   | 5:AX:18:PRO:HD2    | 2.16                     | 0.46              |
| 1:AS:3209:A:OP1   | 5:AX:97:ARG:NH2    | 2.35                     | 0.46              |
| 2:AT:27:A:H2'     | 2:AT:28:C:C6       | 2.50                     | 0.46              |
| 4:AW:204:MET:HB3  | 4:AW:208:ASP:HB2   | 1.96                     | 0.46              |
| 10:BC:116:ALA:HB1 | 10:BC:126:VAL:HG21 | 1.97                     | 0.46              |
| 15:BH:26:LEU:HD11 | 15:BH:87:TRP:CG    | 2.51                     | 0.46              |
| 15:BH:62:LEU:HD21 | 15:BH:77:LYS:HB3   | 1.98                     | 0.46              |
| 16:BI:71:ARG:O    | 16:BI:92:LEU:HB2   | 2.15                     | 0.46              |
| 23:BP:19:VAL:HG13 | 23:BP:28:PHE:CD2   | 2.50                     | 0.46              |
| 23:BP:63:LYS:O    | 23:BP:64:VAL:C     | 2.58                     | 0.46              |
| 46:CM:146:A:H61   | 53:CT:133:LEU:CD1  | 2.28                     | 0.46              |
| 46:CM:1238:U:C2   | 46:CM:1239:U:C5    | 3.03                     | 0.46              |
| 54:CU:71:THR:HB   | 54:CU:127:PHE:CD2  | 2.50                     | 0.46              |
| 59:CZ:62:LEU:HD22 | 59:CZ:71:ILE:HG22  | 1.98                     | 0.46              |
| 63:DD:27:LEU:HB3  | 63:DD:63:ASP:HB2   | 1.97                     | 0.46              |
| 72:DM:90:THR:OG1  | 72:DM:104:ALA:HB2  | 2.16                     | 0.46              |
| 79:DT:20:VAL:HG12 | 79:DT:36:GLY:O     | 2.16                     | 0.46              |
| 79:DT:82:LEU:HA   | 79:DT:82:LEU:HD23  | 1.70                     | 0.46              |
| 79:DT:164:SER:OG  | 79:DT:179:ASP:OD1  | 2.30                     | 0.46              |
| 79:DT:203:PRO:C   | 79:DT:205:GLY:H    | 2.23                     | 0.46              |
| 79:DT:209:ALA:N   | 79:DT:242:PHE:HE1  | 2.09                     | 0.46              |
| 1:1:964:G:H2'     | 1:1:965:C:C6       | 2.51                     | 0.46              |
| 1:1:1444:U:OP1    | 18:x:67:ILE:HG22   | 2.16                     | 0.46              |
| 1:1:1466:U:H2'    | 1:1:1467:U:H6      | 1.80                     | 0.46              |
| 1:1:1486:A:O2'    | 38:AK:12:HIS:O     | 2.31                     | 0.46              |
| 1:1:1593:C:OP1    | 35:AH:8:ARG:NH2    | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1799:C:H4'    | 35:AH:62:TYR:HB3  | 1.98                     | 0.46              |
| 1:1:1825:A:H5''   | 1:1:1826:G:H5'    | 1.96                     | 0.46              |
| 1:1:1859:U:OP2    | 20:z:70:LYS:NZ    | 2.47                     | 0.46              |
| 1:1:2384:C:H2'    | 1:1:2385:C:H6     | 1.79                     | 0.46              |
| 1:1:2458:G:H2'    | 1:1:2458:G:N3     | 2.30                     | 0.46              |
| 1:1:3264:C:H2'    | 1:1:3265:U:H6     | 1.81                     | 0.46              |
| 5:k:112:GLU:HG3   | 5:k:122:TRP:CZ2   | 2.51                     | 0.46              |
| 5:k:159:ARG:HG2   | 5:k:182:GLN:HA    | 1.98                     | 0.46              |
| 8:n:45:ARG:HD3    | 8:n:46:PHE:CZ     | 2.51                     | 0.46              |
| 8:n:59:ASP:OD2    | 8:n:77:ARG:NH1    | 2.48                     | 0.46              |
| 13:s:61:ARG:HH21  | 45:i:43:PRO:HG2   | 1.80                     | 0.46              |
| 16:v:14:LYS:HG2   | 16:v:23:TYR:HE2   | 1.80                     | 0.46              |
| 19:y:64:VAL:HG12  | 19:y:93:LEU:HD11  | 1.97                     | 0.46              |
| 29:AB:63:LYS:HE2  | 29:AB:65:GLN:HE22 | 1.80                     | 0.46              |
| 32:AE:78:ARG:HA   | 32:AE:88:LEU:HD23 | 1.98                     | 0.46              |
| 46:B:446:C:H2'    | 46:B:447:C:C6     | 2.50                     | 0.46              |
| 46:B:904:A:H2'    | 46:B:905:C:C6     | 2.50                     | 0.46              |
| 62:R:81:ARG:HB2   | 62:R:117:GLY:CA   | 2.43                     | 0.46              |
| 1:AS:87:A:H2'     | 1:AS:88:G:O4'     | 2.15                     | 0.46              |
| 1:AS:314:U:H2'    | 1:AS:315:C:H6     | 1.81                     | 0.46              |
| 1:AS:1202:G:OP1   | 80:BE:157:TYR:OH  | 2.28                     | 0.46              |
| 1:AS:1335:C:OP1   | 33:BZ:62:LYS:HB2  | 2.15                     | 0.46              |
| 1:AS:1941:A:H2'   | 1:AS:1942:A:C8    | 2.51                     | 0.46              |
| 1:AS:2790:U:H6    | 1:AS:2790:U:H5'   | 1.81                     | 0.46              |
| 1:AS:3067:U:H2'   | 1:AS:3068:C:C6    | 2.50                     | 0.46              |
| 3:AU:46:G:OP2     | 40:CG:15:LYS:NZ   | 2.41                     | 0.46              |
| 10:BC:99:ARG:HH21 | 10:BC:192:HIS:CD2 | 2.34                     | 0.46              |
| 23:BP:84:LYS:HD3  | 23:BP:93:ARG:HH21 | 1.79                     | 0.46              |
| 27:BT:43:TYR:HD1  | 27:BT:126:ALA:HA  | 1.81                     | 0.46              |
| 36:CC:9:LEU:HD21  | 36:CC:54:VAL:HG22 | 1.96                     | 0.46              |
| 45:CL:164:GLU:HG3 | 45:CL:165:LEU:H   | 1.81                     | 0.46              |
| 46:CM:191:U:H4'   | 46:CM:192:U:H5'   | 1.98                     | 0.46              |
| 46:CM:487:C:O2    | 46:CM:496:G:C2    | 2.69                     | 0.46              |
| 46:CM:1092:G:O2'  | 46:CM:1093:G:H5'  | 2.16                     | 0.46              |
| 46:CM:1221:A:N3   | 78:DS:180:ARG:NH2 | 2.63                     | 0.46              |
| 46:CM:1225:U:H1'  | 46:CM:1229:A:N1   | 2.30                     | 0.46              |
| 46:CM:1341:U:H2'  | 46:CM:1342:A:H8   | 1.81                     | 0.46              |
| 46:CM:1511:A:N3   | 46:CM:1577:G:O2'  | 2.40                     | 0.46              |
| 46:CM:1571:G:H22  | 46:CM:1598:A:P    | 2.37                     | 0.46              |
| 46:CM:1739:U:H2'  | 46:CM:1740:A:C8   | 2.49                     | 0.46              |
| 48:CO:195:ARG:O   | 48:CO:199:LYS:N   | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:CQ:68:HIS:NE2  | 57:CX:94:ASN:HB3  | 2.31                     | 0.46              |
| 50:CQ:172:ALA:HB1 | 50:CQ:174:ARG:NH1 | 2.31                     | 0.46              |
| 70:DK:133:LEU:HG  | 70:DK:137:LYS:HD2 | 1.97                     | 0.46              |
| 72:DM:60:VAL:HG23 | 72:DM:101:TYR:HB2 | 1.98                     | 0.46              |
| 72:DM:74:SER:HA   | 72:DM:77:ARG:NH2  | 2.30                     | 0.46              |
| 78:DS:142:LEU:O   | 78:DS:143:ALA:HB3 | 2.16                     | 0.46              |
| 81:P0:12:PHE:CD1  | 81:P0:12:PHE:N    | 2.82                     | 0.46              |
| 1:1:58:G:H2'      | 3:4:33:A:O2'      | 2.15                     | 0.46              |
| 1:1:130:U:H2'     | 1:1:131:C:C6      | 2.51                     | 0.46              |
| 1:1:386:A:C5      | 1:1:387:A:H1'     | 2.50                     | 0.46              |
| 1:1:559:C:H2'     | 1:1:560:C:C6      | 2.49                     | 0.46              |
| 1:1:3023:U:C2     | 1:1:3024:G:C8     | 3.04                     | 0.46              |
| 1:1:3126:U:C5     | 1:1:3128:G:C2     | 3.04                     | 0.46              |
| 3:4:97:A:OP1      | 36:AI:63:ARG:NH2  | 2.47                     | 0.46              |
| 8:n:135:VAL:O     | 8:n:139:LYS:HD3   | 2.14                     | 0.46              |
| 31:AD:18:LEU:HB3  | 31:AD:100:SER:HB2 | 1.97                     | 0.46              |
| 39:AL:24:ILE:HD13 | 39:AL:76:THR:HB   | 1.98                     | 0.46              |
| 42:AO:18:ARG:NH2  | 46:B:1111:G:OP2   | 2.49                     | 0.46              |
| 45:i:62:ALA:O     | 45:i:63:ALA:C     | 2.59                     | 0.46              |
| 46:B:1:U:C2       | 46:B:3:U:C4       | 3.04                     | 0.46              |
| 46:B:121:U:O2'    | 51:G:33:ALA:O     | 2.31                     | 0.46              |
| 46:B:331:A:OP2    | 55:K:31:ARG:NH1   | 2.40                     | 0.46              |
| 46:B:445:U:H2'    | 46:B:446:C:O4'    | 2.16                     | 0.46              |
| 46:B:585:C:H2'    | 46:B:586:U:C6     | 2.51                     | 0.46              |
| 46:B:653:G:N2     | 46:B:676:G:N7     | 2.63                     | 0.46              |
| 46:B:848:A:H2'    | 46:B:850:A:C2     | 2.51                     | 0.46              |
| 46:B:1239:U:OP2   | 59:O:46:ARG:NH1   | 2.47                     | 0.46              |
| 49:E:148:SER:OG   | 49:E:149:LEU:N    | 2.49                     | 0.46              |
| 52:H:145:ASP:OD1  | 52:H:146:SER:N    | 2.49                     | 0.46              |
| 54:J:134:LYS:HG3  | 60:P:18:TYR:OH    | 2.16                     | 0.46              |
| 59:O:32:LEU:HD23  | 59:O:32:LEU:HA    | 1.76                     | 0.46              |
| 79:AR:40:LYS:HD2  | 79:AR:65:HIS:O    | 2.15                     | 0.46              |
| 1:AS:757:A:H2'    | 1:AS:758:U:C6     | 2.51                     | 0.46              |
| 1:AS:762:U:H4'    | 1:AS:763:U:O4'    | 2.15                     | 0.46              |
| 1:AS:1099:A:OP2   | 1:AS:1100:G:H5'   | 2.16                     | 0.46              |
| 1:AS:1302:G:C5    | 17:BJ:63:THR:HA   | 2.51                     | 0.46              |
| 1:AS:1661:U:H2'   | 1:AS:1662:G:C8    | 2.51                     | 0.46              |
| 1:AS:1746:A:O5'   | 39:CF:26:LYS:HE3  | 2.16                     | 0.46              |
| 1:AS:1753:G:H4'   | 23:BP:99:VAL:HG13 | 1.97                     | 0.46              |
| 1:AS:2079:C:HO2'  | 1:AS:2080:U:H6    | 1.62                     | 0.46              |
| 1:AS:2527:G:N2    | 1:AS:2527:G:OP2   | 2.49                     | 0.46              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:AT:59:U:H2'     | 2:AT:60:G:H8        | 1.81                     | 0.46              |
| 19:BL:133:LYS:HB2 | 19:BL:135:GLN:NE2   | 2.31                     | 0.46              |
| 19:BL:150:VAL:HA  | 19:BL:153:PHE:CD2   | 2.50                     | 0.46              |
| 20:BM:114:LYS:O   | 20:BM:146:LYS:NZ    | 2.48                     | 0.46              |
| 20:BM:163:ARG:HD3 | 46:CM:797:U:O2      | 2.16                     | 0.46              |
| 22:BO:97:LYS:HB3  | 22:BO:97:LYS:HE2    | 1.65                     | 0.46              |
| 23:BP:92:ILE:HA   | 23:BP:95:TRP:CZ3    | 2.51                     | 0.46              |
| 36:CC:34:GLN:O    | 36:CC:38:ARG:HB2    | 2.16                     | 0.46              |
| 43:CJ:8:ARG:HG2   | 43:CJ:10:THR:HG23   | 1.97                     | 0.46              |
| 45:CL:42:ALA:O    | 45:CL:43:PRO:C      | 2.59                     | 0.46              |
| 46:CM:504:A:H5''  | 46:CM:505:U:P       | 2.56                     | 0.46              |
| 46:CM:824:U:C2    | 46:CM:825:U:C4      | 3.04                     | 0.46              |
| 46:CM:1470:G:H2'  | 46:CM:1471:C:C6     | 2.51                     | 0.46              |
| 46:CM:1573:A:H2'  | 46:CM:1574:A:O4'    | 2.15                     | 0.46              |
| 46:CM:1629:G:OP2  | 86:CM:1822:GET:H832 | 2.15                     | 0.46              |
| 57:CX:38:ARG:HB2  | 57:CX:41:PHE:CD2    | 2.51                     | 0.46              |
| 79:DT:261:LYS:HE2 | 79:DT:266:SER:CB    | 2.45                     | 0.46              |
| 1:1:216:U:H4'     | 27:9:100:HIS:CD2    | 2.51                     | 0.46              |
| 1:1:595:G:H21     | 6:l:323:GLN:CD      | 2.24                     | 0.46              |
| 1:1:1218:G:OP1    | 81:P0:55:LYS:CD     | 2.64                     | 0.46              |
| 1:1:1923:G:C8     | 44:AQ:16:VAL:HA     | 2.51                     | 0.46              |
| 1:1:3021:A:N3     | 5:k:55:THR:OG1      | 2.44                     | 0.46              |
| 1:1:3318:G:O5'    | 55:K:77:ARG:NH2     | 2.29                     | 0.46              |
| 25:7:91:LYS:HB2   | 25:7:91:LYS:HE3     | 1.78                     | 0.46              |
| 45:i:67:LYS:HD3   | 45:i:67:LYS:HA      | 1.74                     | 0.46              |
| 46:B:86:A:H5'     | 71:a:119:PHE:CE1    | 2.51                     | 0.46              |
| 46:B:165:U:H2'    | 46:B:166:A:H5''     | 1.97                     | 0.46              |
| 46:B:480:U:C2     | 46:B:481:A:C8       | 3.04                     | 0.46              |
| 49:E:155:GLY:N    | 49:E:212:ALA:HB2    | 2.31                     | 0.46              |
| 52:H:80:LYS:HB2   | 52:H:83:ARG:NH1     | 2.30                     | 0.46              |
| 62:R:77:LYS:HB3   | 62:R:102:PHE:HE1    | 1.77                     | 0.46              |
| 1:AS:99:A:H3'     | 1:AS:100:G:H21      | 1.81                     | 0.46              |
| 1:AS:224:C:OP1    | 27:BT:47:SER:OG     | 2.33                     | 0.46              |
| 1:AS:378:A:H1'    | 27:BT:90:SER:O      | 2.16                     | 0.46              |
| 1:AS:546:C:H2'    | 1:AS:547:U:O4'      | 2.16                     | 0.46              |
| 2:AT:96:U:H4'     | 21:BN:119:ARG:HB2   | 1.96                     | 0.46              |
| 4:AW:112:ILE:HG13 | 44:CK:79:VAL:HG22   | 1.97                     | 0.46              |
| 5:AX:4:ARG:HD3    | 5:AX:7:GLU:HG2      | 1.98                     | 0.46              |
| 6:AY:141:HIS:HA   | 6:AY:178:ASP:OD1    | 2.16                     | 0.46              |
| 22:BO:108:ARG:CZ  | 22:BO:130:ARG:HH12  | 2.29                     | 0.46              |
| 26:BS:49:LYS:HA   | 36:CC:79:ASP:OD1    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 46:CM:1537:A:H2'  | 46:CM:1538:U:C6     | 2.50                     | 0.46              |
| 46:CM:1744:G:N7   | 86:CM:1822:GET:H222 | 2.31                     | 0.46              |
| 53:CT:220:LYS:HD2 | 53:CT:223:ARG:HH21  | 1.81                     | 0.46              |
| 59:CZ:137:LEU:O   | 59:CZ:141:SER:HB3   | 2.16                     | 0.46              |
| 62:DC:108:LYS:HD2 | 62:DC:111:MET:HE3   | 1.98                     | 0.46              |
| 63:DD:25:LYS:O    | 63:DD:63:ASP:HB3    | 2.15                     | 0.46              |
| 64:DE:81:LYS:N    | 64:DE:83:GLN:OE1    | 2.49                     | 0.46              |
| 78:DS:147:TYR:CD1 | 78:DS:147:TYR:N     | 2.84                     | 0.46              |
| 1:1:671:U:H2'     | 1:1:672:G:H8        | 1.80                     | 0.45              |
| 1:1:818:G:H2'     | 1:1:819:C:H6        | 1.81                     | 0.45              |
| 1:1:903:G:C4      | 1:1:922:A:C8        | 3.03                     | 0.45              |
| 1:1:1592:C:H2'    | 1:1:1593:C:C6       | 2.52                     | 0.45              |
| 1:1:2077:A:O2'    | 1:1:2078:A:H5'      | 2.16                     | 0.45              |
| 1:1:3268:G:H3'    | 1:1:3342:G:O4'      | 2.16                     | 0.45              |
| 3:4:142:C:H2'     | 3:4:143:U:C6        | 2.51                     | 0.45              |
| 10:p:201:LEU:HD21 | 10:p:204:VAL:HG13   | 1.96                     | 0.45              |
| 10:p:202:THR:O    | 10:p:203:GLU:HG2    | 2.17                     | 0.45              |
| 19:y:133:LYS:HB2  | 19:y:135:GLN:NE2    | 2.30                     | 0.45              |
| 31:AD:53:LEU:HD22 | 35:AH:91:ARG:CZ     | 2.47                     | 0.45              |
| 45:i:99:SER:OG    | 46:B:574:G:OP2      | 2.28                     | 0.45              |
| 46:B:152:G:O2'    | 53:I:60:GLY:HA2     | 2.15                     | 0.45              |
| 46:B:160:A:H3'    | 46:B:161:G:H21      | 1.81                     | 0.45              |
| 46:B:1485:G:H2'   | 46:B:1486:G:C8      | 2.51                     | 0.45              |
| 46:B:1776:G:OP1   | 73:c:17:HIS:NE2     | 2.40                     | 0.45              |
| 55:K:158:ILE:HG22 | 58:N:24:LYS:HD2     | 1.98                     | 0.45              |
| 57:M:27:PHE:O     | 57:M:40:LEU:HB2     | 2.16                     | 0.45              |
| 65:U:22:ILE:HD11  | 65:U:35:ILE:HD11    | 1.98                     | 0.45              |
| 66:V:15:ILE:HG23  | 66:V:59:ALA:HB3     | 1.97                     | 0.45              |
| 70:Z:59:ILE:HG23  | 77:g:4:VAL:HG22     | 1.97                     | 0.45              |
| 1:AS:29:G:H5''    | 16:BI:188:ARG:NH1   | 2.31                     | 0.45              |
| 1:AS:1434:U:H2'   | 1:AS:1435:U:C6      | 2.50                     | 0.45              |
| 1:AS:1656:C:H2'   | 1:AS:1657:G:C8      | 2.50                     | 0.45              |
| 1:AS:1706:C:H2'   | 1:AS:1707:U:H6      | 1.81                     | 0.45              |
| 1:AS:1714:G:OP1   | 20:BM:118:HIS:HA    | 2.16                     | 0.45              |
| 1:AS:2332:C:H2'   | 1:AS:2333:G:O4'     | 2.16                     | 0.45              |
| 1:AS:2650:A:H8    | 45:CL:56:SER:HB2    | 1.81                     | 0.45              |
| 1:AS:2717:G:N2    | 1:AS:2719:A:H3'     | 2.30                     | 0.45              |
| 1:AS:2777:G:O2'   | 1:AS:2939:A:N1      | 2.43                     | 0.45              |
| 9:BB:135:GLY:N    | 9:BB:233:ILE:HD12   | 2.32                     | 0.45              |
| 27:BT:47:SER:O    | 27:BT:122:LYS:HE2   | 2.16                     | 0.45              |
| 28:BU:23:VAL:HA   | 28:BU:45:GLY:HA2    | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:CF:71:PRO:O     | 39:CF:72:THR:C     | 2.59                     | 0.45              |
| 43:CJ:72:LEU:O     | 43:CJ:80:LYS:HA    | 2.16                     | 0.45              |
| 46:CM:166:A:H2'    | 46:CM:167:A:C8     | 2.51                     | 0.45              |
| 46:CM:520:U:O3'    | 71:DL:60:PHE:HB2   | 2.16                     | 0.45              |
| 46:CM:641:G:N1     | 46:CM:690:C:N3     | 2.64                     | 0.45              |
| 46:CM:654:G:O5'    | 46:CM:654:G:C8     | 2.68                     | 0.45              |
| 46:CM:824:U:N3     | 46:CM:825:U:C4     | 2.83                     | 0.45              |
| 46:CM:961:G:N1     | 46:CM:1008:A:O2'   | 2.34                     | 0.45              |
| 46:CM:1446:A:H5''  | 62:DC:128:HIS:CE1  | 2.51                     | 0.45              |
| 46:CM:1742:A:C4    | 46:CM:1743:A:C8    | 3.04                     | 0.45              |
| 48:CO:140:ILE:HG22 | 48:CO:211:HIS:O    | 2.17                     | 0.45              |
| 51:CR:36:HIS:CG    | 51:CR:85:GLY:HA3   | 2.51                     | 0.45              |
| 54:CU:5:ILE:HD13   | 54:CU:15:LEU:HD23  | 1.98                     | 0.45              |
| 60:DA:95:ALA:O     | 60:DA:99:ARG:HG2   | 2.15                     | 0.45              |
| 71:DL:63:GLN:CD    | 71:DL:68:LYS:HD3   | 2.41                     | 0.45              |
| 72:DM:61:SER:H     | 72:DM:64:VAL:HB    | 1.81                     | 0.45              |
| 78:DS:147:TYR:HB2  | 78:DS:148:TYR:CD1  | 2.51                     | 0.45              |
| 79:DT:169:ALA:CB   | 79:DT:175:VAL:HG22 | 2.41                     | 0.45              |
| 81:P0:66:PHE:C     | 81:P0:68:SER:H     | 2.24                     | 0.45              |
| 1:1:147:G:H5''     | 16:v:55:ALA:CB     | 2.45                     | 0.45              |
| 1:1:596:G:C2       | 1:1:597:U:C2       | 3.04                     | 0.45              |
| 1:1:624:U:H2'      | 1:1:625:C:H6       | 1.81                     | 0.45              |
| 1:1:929:A:C2       | 6:l:99:ARG:NH2     | 2.84                     | 0.45              |
| 1:1:2081:U:H2'     | 1:1:2082:A:H8      | 1.82                     | 0.45              |
| 1:1:2203:U:H2'     | 1:1:2204:U:C6      | 2.50                     | 0.45              |
| 1:1:2410:A:C2      | 16:v:125:SER:HB2   | 2.51                     | 0.45              |
| 1:1:2411:U:H1'     | 16:v:125:SER:HB3   | 1.99                     | 0.45              |
| 1:1:2628:A:C8      | 1:1:2630:G:C8      | 3.05                     | 0.45              |
| 1:1:3038:U:H2'     | 1:1:3039:C:H6      | 1.81                     | 0.45              |
| 1:1:3197:G:H2'     | 1:1:3198:C:C6      | 2.51                     | 0.45              |
| 1:1:3259:A:H2'     | 1:1:3260:A:O4'     | 2.17                     | 0.45              |
| 4:j:70:LYS:HG3     | 4:j:71:LEU:N       | 2.30                     | 0.45              |
| 21:0:27:MET:HE2    | 21:0:27:MET:HB3    | 1.81                     | 0.45              |
| 25:7:105:ARG:O     | 25:7:109:LEU:HG    | 2.15                     | 0.45              |
| 46:B:184:C:P       | 55:K:152:ARG:HH22  | 2.37                     | 0.45              |
| 46:B:471:A:H2'     | 46:B:472:A:O4'     | 2.15                     | 0.45              |
| 46:B:836:U:H2'     | 46:B:837:C:C6      | 2.52                     | 0.45              |
| 46:B:1220:C:H3'    | 46:B:1221:A:H8     | 1.80                     | 0.45              |
| 51:G:103:TYR:CD1   | 51:G:189:LEU:HD21  | 2.51                     | 0.45              |
| 59:O:55:ARG:HH12   | 59:O:82:PRO:HD3    | 1.81                     | 0.45              |
| 59:O:97:LEU:HA     | 59:O:100:TRP:CZ2   | 2.52                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:R:96:VAL:HG13  | 62:R:120:SER:OG    | 2.16                     | 0.45              |
| 79:AR:257:ILE:O   | 79:AR:271:LEU:N    | 2.48                     | 0.45              |
| 1:AS:284:A:C5     | 43:CJ:41:ARG:NH1   | 2.84                     | 0.45              |
| 1:AS:798:C:H2'    | 1:AS:799:C:H6      | 1.80                     | 0.45              |
| 1:AS:859:C:H2'    | 1:AS:860:G:O4'     | 2.16                     | 0.45              |
| 1:AS:1099:A:N6    | 1:AS:1359:A:H1'    | 2.31                     | 0.45              |
| 1:AS:1286:A:H2'   | 1:AS:1287:A:C8     | 2.51                     | 0.45              |
| 1:AS:1416:C:OP1   | 3:AU:20:U:H5''     | 2.17                     | 0.45              |
| 1:AS:1753:G:H4'   | 23:BP:99:VAL:CG1   | 2.46                     | 0.45              |
| 1:AS:2328:C:O3'   | 18:BK:68:GLY:HA3   | 2.16                     | 0.45              |
| 1:AS:2502:A:H1'   | 1:AS:2503:G:C8     | 2.52                     | 0.45              |
| 1:AS:2603:U:H2'   | 1:AS:2604:G:H8     | 1.81                     | 0.45              |
| 1:AS:2614:A:H2'   | 1:AS:2615:A:C8     | 2.50                     | 0.45              |
| 1:AS:2672:G:H5''  | 22:BO:17:ARG:HG2   | 1.98                     | 0.45              |
| 3:AU:79:A:O2'     | 36:CC:43:ARG:NH1   | 2.49                     | 0.45              |
| 14:BG:59:ARG:HH12 | 14:BG:68:LYS:C     | 2.24                     | 0.45              |
| 23:BP:17:VAL:CG2  | 23:BP:64:VAL:HB    | 2.46                     | 0.45              |
| 23:BP:60:SER:O    | 23:BP:63:LYS:HG3   | 2.17                     | 0.45              |
| 26:BS:66:PRO:HA   | 26:BS:84:PHE:HD1   | 1.82                     | 0.45              |
| 46:CM:498:C:C2    | 46:CM:499:U:C6     | 3.04                     | 0.45              |
| 46:CM:849:U:O2    | 74:DO:21:LEU:HB3   | 2.15                     | 0.45              |
| 46:CM:1551:U:H2'  | 46:CM:1552:C:H6    | 1.81                     | 0.45              |
| 46:CM:1712:U:H2'  | 46:CM:1713:G:C8    | 2.51                     | 0.45              |
| 51:CR:45:VAL:HA   | 51:CR:61:VAL:HG21  | 1.97                     | 0.45              |
| 52:CS:27:THR:OG1  | 63:DD:27:LEU:HA    | 2.17                     | 0.45              |
| 52:CS:80:LYS:HA   | 52:CS:80:LYS:HD3   | 1.76                     | 0.45              |
| 52:CS:100:ASN:O   | 52:CS:101:GLY:C    | 2.58                     | 0.45              |
| 53:CT:234:LEU:HG  | 53:CT:235:LYS:CD   | 2.46                     | 0.45              |
| 54:CU:52:LYS:HE2  | 54:CU:84:ARG:CZ    | 2.46                     | 0.45              |
| 54:CU:166:GLN:HG3 | 54:CU:179:PHE:HD2  | 1.81                     | 0.45              |
| 56:CW:37:LYS:HA   | 77:DR:33:ARG:HA    | 1.99                     | 0.45              |
| 69:DJ:40:VAL:HG11 | 69:DJ:103:ILE:HD12 | 1.97                     | 0.45              |
| 1:1:98:A:OP1      | 16:v:194:HIS:HB3   | 2.16                     | 0.45              |
| 1:1:483:U:H2'     | 1:1:484:U:H6       | 1.76                     | 0.45              |
| 1:1:1021:A:H8     | 1:1:1021:A:OP1     | 2.00                     | 0.45              |
| 1:1:1221:A:H2'    | 1:1:1222:G:C8      | 2.51                     | 0.45              |
| 1:1:1269:A:C2     | 1:1:1270:A:H1'     | 2.52                     | 0.45              |
| 1:1:1621:A:H4'    | 1:1:1639:A:C5      | 2.51                     | 0.45              |
| 1:1:2327:U:O2'    | 1:1:3272:A:N3      | 2.48                     | 0.45              |
| 1:1:2478:A:N3     | 1:1:2478:A:H2'     | 2.30                     | 0.45              |
| 6:l:113:LYS:HG3   | 16:v:202:TYR:HB3   | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:w:35:VAL:HG22   | 17:w:104:LYS:HB2   | 1.98                     | 0.45              |
| 25:7:47:ARG:HD2    | 25:7:58:HIS:CE1    | 2.51                     | 0.45              |
| 25:7:115:ALA:O     | 25:7:118:ALA:HB3   | 2.16                     | 0.45              |
| 31:AD:43:LEU:HD23  | 31:AD:94:ILE:HD12  | 1.98                     | 0.45              |
| 46:B:397:A:H1'     | 46:B:399:A:O4'     | 2.16                     | 0.45              |
| 46:B:788:A:C8      | 69:Y:107:SER:HA    | 2.51                     | 0.45              |
| 46:B:913:U:OP1     | 73:c:19:LYS:HE3    | 2.16                     | 0.45              |
| 46:B:1551:U:H2'    | 46:B:1552:C:H6     | 1.81                     | 0.45              |
| 47:C:18:LEU:HD22   | 64:T:102:ILE:HG21  | 1.98                     | 0.45              |
| 1:AS:297:G:H5''    | 37:CD:84:ARG:HH21  | 1.81                     | 0.45              |
| 1:AS:976:A:C2'     | 1:AS:977:U:H5'     | 2.45                     | 0.45              |
| 3:AU:6:U:H2'       | 3:AU:7:U:C6        | 2.51                     | 0.45              |
| 7:AZ:235:ASP:OD1   | 7:AZ:235:ASP:N     | 2.44                     | 0.45              |
| 14:BG:32:LYS:HG2   | 14:BG:35:ARG:NH2   | 2.28                     | 0.45              |
| 22:BO:16:GLN:HG2   | 22:BO:17:ARG:O     | 2.16                     | 0.45              |
| 34:CA:53:TYR:CZ    | 34:CA:65:ARG:HB2   | 2.52                     | 0.45              |
| 45:CL:55:LYS:O     | 45:CL:56:SER:C     | 2.58                     | 0.45              |
| 45:CL:155:LEU:HD13 | 57:CX:92:LEU:CD1   | 2.41                     | 0.45              |
| 46:CM:443:A:H1'    | 46:CM:523:A:H5'    | 1.98                     | 0.45              |
| 46:CM:846:U:O2'    | 69:DJ:56:HIS:O     | 2.28                     | 0.45              |
| 46:CM:1149:G:H2'   | 46:CM:1150:G:C8    | 2.51                     | 0.45              |
| 46:CM:1160:U:H2'   | 46:CM:1161:G:C8    | 2.50                     | 0.45              |
| 46:CM:1213:G:OP1   | 59:CZ:118:ALA:HA   | 2.16                     | 0.45              |
| 46:CM:1278:U:OP2   | 49:CP:111:LYS:NZ   | 2.47                     | 0.45              |
| 46:CM:1537:A:OP2   | 62:DC:42:ARG:NH2   | 2.50                     | 0.45              |
| 46:CM:1763:A:H2'   | 46:CM:1764:G:H8    | 1.80                     | 0.45              |
| 48:CO:31:ASP:OD1   | 48:CO:45:LYS:HB2   | 2.17                     | 0.45              |
| 48:CO:43:VAL:HG23  | 48:CO:44:GLY:N     | 2.31                     | 0.45              |
| 48:CO:115:ARG:N    | 48:CO:118:GLN:OE1  | 2.42                     | 0.45              |
| 48:CO:183:GLN:O    | 48:CO:187:LYS:HB2  | 2.17                     | 0.45              |
| 50:CQ:214:ASP:OD1  | 50:CQ:215:GLU:N    | 2.30                     | 0.45              |
| 53:CT:48:TYR:OH    | 53:CT:121:ILE:HG12 | 2.15                     | 0.45              |
| 54:CU:161:LYS:HB2  | 54:CU:165:PHE:CE2  | 2.51                     | 0.45              |
| 62:DC:50:ASP:OD2   | 62:DC:53:PRO:HD3   | 2.16                     | 0.45              |
| 79:DT:9:LEU:HB2    | 79:DT:310:TRP:CH2  | 2.52                     | 0.45              |
| 79:DT:23:LEU:HD22  | 79:DT:33:LEU:CD2   | 2.47                     | 0.45              |
| 79:DT:124:VAL:HA   | 79:DT:133:LYS:O    | 2.16                     | 0.45              |
| 1:1:75:G:H3'       | 14:t:73:ARG:HD2    | 1.97                     | 0.45              |
| 1:1:115:A:OP2      | 16:v:2:GLY:N       | 2.49                     | 0.45              |
| 1:1:260:C:H2'      | 1:1:261:U:C6       | 2.51                     | 0.45              |
| 1:1:952:U:H2'      | 1:1:953:C:C6       | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1011:C:HO2'   | 1:1:1012:U:P      | 2.39                     | 0.45              |
| 1:1:1174:G:N3     | 1:1:1324:U:O2'    | 2.49                     | 0.45              |
| 1:1:1286:A:H2'    | 1:1:1287:A:C8     | 2.52                     | 0.45              |
| 1:1:2201:A:H2'    | 1:1:2202:A:C8     | 2.51                     | 0.45              |
| 1:1:2717:G:N2     | 1:1:2719:A:H3'    | 2.31                     | 0.45              |
| 1:1:2956:C:H2'    | 1:1:2957:C:H6     | 1.82                     | 0.45              |
| 1:1:3162:U:H4'    | 1:1:3162:U:OP1    | 2.16                     | 0.45              |
| 7:m:41:LYS:HD3    | 7:m:41:LYS:HA     | 1.79                     | 0.45              |
| 22:2:44:ALA:HB2   | 22:2:53:PRO:HG2   | 1.98                     | 0.45              |
| 22:2:80:VAL:O     | 22:2:83:ARG:NH1   | 2.49                     | 0.45              |
| 34:AG:103:TYR:HA  | 34:AG:105:SER:N   | 2.32                     | 0.45              |
| 46:B:289:G:H2'    | 46:B:290:U:C6     | 2.52                     | 0.45              |
| 46:B:1344:C:O2    | 66:V:3:GLY:HA3    | 2.16                     | 0.45              |
| 46:B:1589:C:H2'   | 46:B:1590:U:C6    | 2.52                     | 0.45              |
| 48:D:59:ASP:OD1   | 48:D:60:GLY:N     | 2.49                     | 0.45              |
| 48:D:82:ARG:NH2   | 48:D:188:LEU:O    | 2.48                     | 0.45              |
| 70:Z:133:LEU:HG   | 70:Z:137:LYS:HD2  | 1.98                     | 0.45              |
| 1:AS:15:A:H2'     | 1:AS:16:G:O4'     | 2.16                     | 0.45              |
| 1:AS:148:U:H4'    | 16:BI:56:LYS:HG2  | 1.99                     | 0.45              |
| 1:AS:234:A:H2'    | 1:AS:235:G:O4'    | 2.16                     | 0.45              |
| 1:AS:429:U:H4'    | 34:CA:88:ASN:O    | 2.16                     | 0.45              |
| 1:AS:851:U:H4'    | 20:BM:95:TRP:CE2  | 2.51                     | 0.45              |
| 1:AS:907:C:OP2    | 4:AW:9:ARG:HD2    | 2.16                     | 0.45              |
| 1:AS:1377:A:H2'   | 1:AS:1378:G:H8    | 1.80                     | 0.45              |
| 1:AS:1791:U:H2'   | 4:AW:50:HIS:HD2   | 1.80                     | 0.45              |
| 1:AS:2738:U:H2'   | 1:AS:2739:U:H6    | 1.82                     | 0.45              |
| 1:AS:3165:U:H2'   | 1:AS:3166:A:C4'   | 2.46                     | 0.45              |
| 3:AU:75:G:H2'     | 3:AU:76:C:C6      | 2.50                     | 0.45              |
| 5:AX:123:TYR:CZ   | 5:AX:124:LYS:HG3  | 2.51                     | 0.45              |
| 10:BC:227:TYR:O   | 10:BC:231:ARG:HG3 | 2.17                     | 0.45              |
| 15:BH:111:PHE:O   | 15:BH:114:MET:HB3 | 2.17                     | 0.45              |
| 19:BL:158:HIS:CD2 | 19:BL:186:VAL:HA  | 2.52                     | 0.45              |
| 26:BS:47:GLN:HE22 | 26:BS:49:LYS:HG2  | 1.81                     | 0.45              |
| 46:CM:497:U:C2    | 46:CM:498:C:C5    | 3.04                     | 0.45              |
| 46:CM:809:G:H2'   | 46:CM:810:U:C6    | 2.52                     | 0.45              |
| 46:CM:938:G:H2'   | 46:CM:939:G:H8    | 1.82                     | 0.45              |
| 46:CM:1376:U:C5   | 64:DE:3:ARG:HG3   | 2.52                     | 0.45              |
| 46:CM:1445:C:H2'  | 65:DF:138:THR:OG1 | 2.16                     | 0.45              |
| 46:CM:1512:A:H2'  | 46:CM:1513:A:C8   | 2.52                     | 0.45              |
| 57:CX:50:THR:HG23 | 57:CX:55:VAL:O    | 2.17                     | 0.45              |
| 79:DT:5:GLU:HG3   | 79:DT:246:ARG:CZ  | 2.46                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:429:U:H4'     | 34:AG:88:ASN:O     | 2.16                     | 0.45              |
| 1:1:780:A:O2'     | 1:1:781:G:OP2      | 2.33                     | 0.45              |
| 1:1:1079:G:H2'    | 1:1:1080:A:H8      | 1.82                     | 0.45              |
| 1:1:1221:A:H2'    | 1:1:1222:G:H8      | 1.81                     | 0.45              |
| 1:1:1278:G:O3'    | 81:P0:82:GLY:HA2   | 2.16                     | 0.45              |
| 1:1:1434:U:H2'    | 1:1:1435:U:C6      | 2.51                     | 0.45              |
| 1:1:1705:C:H2'    | 1:1:1706:C:C6      | 2.51                     | 0.45              |
| 1:1:1801:C:O2'    | 35:AH:76:TYR:HA    | 2.17                     | 0.45              |
| 1:1:2210:A:H1'    | 1:1:2407:G:H5'     | 1.98                     | 0.45              |
| 1:1:2581:A:H2'    | 1:1:2582:G:C8      | 2.51                     | 0.45              |
| 1:1:2854:U:H2'    | 1:1:2855:U:H6      | 1.80                     | 0.45              |
| 3:4:119:C:H2'     | 3:4:120:U:H6       | 1.81                     | 0.45              |
| 9:o:36:LYS:HE2    | 9:o:36:LYS:HB2     | 1.80                     | 0.45              |
| 24:6:121:GLU:OE1  | 24:6:121:GLU:N     | 2.49                     | 0.45              |
| 32:AE:95:VAL:HG12 | 32:AE:97:VAL:HG13  | 1.98                     | 0.45              |
| 46:B:4:C:OP1      | 49:E:195:SER:OG    | 2.26                     | 0.45              |
| 46:B:94:U:H2'     | 46:B:95:G:O4'      | 2.16                     | 0.45              |
| 46:B:569:G:H5''   | 70:Z:114:LYS:HE2   | 1.98                     | 0.45              |
| 46:B:887:G:H2'    | 46:B:888:U:C6      | 2.51                     | 0.45              |
| 46:B:1127:A:H2'   | 46:B:1128:A:C8     | 2.52                     | 0.45              |
| 52:H:109:LYS:HG3  | 52:H:112:ARG:HH21  | 1.82                     | 0.45              |
| 63:S:37:LEU:HA    | 63:S:44:ARG:HH21   | 1.80                     | 0.45              |
| 63:S:113:LYS:HG2  | 63:S:117:VAL:HB    | 1.99                     | 0.45              |
| 1:AS:158:A:H2'    | 1:AS:159:A:C8      | 2.51                     | 0.45              |
| 1:AS:374:A:N3     | 1:AS:376:G:H5''    | 2.31                     | 0.45              |
| 1:AS:379:C:H2'    | 1:AS:380:U:C6      | 2.51                     | 0.45              |
| 1:AS:725:G:N2     | 19:BL:139:ILE:HB   | 2.31                     | 0.45              |
| 1:AS:1028:C:H2'   | 1:AS:1029:U:O4'    | 2.17                     | 0.45              |
| 1:AS:1283:A:OP2   | 1:AS:1283:A:H8     | 1.99                     | 0.45              |
| 1:AS:2156:A:H5''  | 4:AW:129:THR:OG1   | 2.15                     | 0.45              |
| 1:AS:2933:G:H2'   | 1:AS:2934:U:C6     | 2.51                     | 0.45              |
| 1:AS:3318:G:C2    | 1:AS:3321:G:C4     | 3.05                     | 0.45              |
| 4:AW:47:GLN:HG2   | 4:AW:49:ILE:HG23   | 1.98                     | 0.45              |
| 21:BN:125:LYS:HG2 | 21:BN:127:VAL:HG23 | 1.99                     | 0.45              |
| 22:BO:45:ASN:H    | 22:BO:95:HIS:CD2   | 2.35                     | 0.45              |
| 27:BT:48:LEU:HD13 | 27:BT:115:ARG:HH21 | 1.81                     | 0.45              |
| 46:CM:815:U:O2'   | 46:CM:816:U:O5'    | 2.35                     | 0.45              |
| 46:CM:1474:G:H3'  | 46:CM:1502:A:H61   | 1.81                     | 0.45              |
| 46:CM:1494:G:H2'  | 46:CM:1495:U:C6    | 2.52                     | 0.45              |
| 46:CM:1543:A:H1'  | 46:CM:1547:U:OP2   | 2.16                     | 0.45              |
| 46:CM:1725:U:H2'  | 46:CM:1726:C:H6    | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:CR:158:ASP:OD1  | 51:CR:175:PHE:N    | 2.43                     | 0.45              |
| 54:CU:30:LEU:HD23  | 54:CU:30:LEU:N     | 2.32                     | 0.45              |
| 57:CX:5:LYS:NZ     | 59:CZ:43:ARG:NH2   | 2.65                     | 0.45              |
| 64:DE:7:LYS:HG3    | 64:DE:8:THR:N      | 2.31                     | 0.45              |
| 78:DS:174:MET:CE   | 78:DS:190:LEU:HD23 | 2.44                     | 0.45              |
| 79:DT:22:SER:HB3   | 79:DT:70:GLN:O     | 2.17                     | 0.45              |
| 79:DT:33:LEU:O     | 79:DT:45:TRP:HB2   | 2.17                     | 0.45              |
| 1:1:377:A:H1'      | 1:1:392:G:N2       | 2.32                     | 0.45              |
| 1:1:2322:U:C1'     | 1:1:3051:C:H41     | 2.30                     | 0.45              |
| 1:1:2546:U:H5'     | 1:1:2547:G:O4'     | 2.16                     | 0.45              |
| 1:1:3005:A:H2'     | 1:1:3006:C:H6      | 1.82                     | 0.45              |
| 1:1:3190:C:H2'     | 1:1:3191:A:H8      | 1.81                     | 0.45              |
| 3:4:38:U:HO2'      | 36:AI:83:LYS:HZ3   | 1.59                     | 0.45              |
| 14:t:126:PHE:CE2   | 14:t:135:VAL:HG22  | 2.51                     | 0.45              |
| 48:D:115:ARG:HA    | 48:D:115:ARG:HD3   | 1.68                     | 0.45              |
| 75:e:35:ASP:O      | 75:e:37:SER:N      | 2.48                     | 0.45              |
| 79:AR:240:LEU:HD22 | 79:AR:249:LEU:HD11 | 1.98                     | 0.45              |
| 1:AS:37:U:H2'      | 1:AS:38:A:O4'      | 2.16                     | 0.45              |
| 1:AS:134:U:H1'     | 36:CC:93:THR:HB    | 1.99                     | 0.45              |
| 1:AS:677:U:H2'     | 1:AS:678:G:C8      | 2.52                     | 0.45              |
| 1:AS:1456:A:H2'    | 1:AS:1457:A:H8     | 1.78                     | 0.45              |
| 1:AS:1530:A:H2'    | 1:AS:1531:A:C8     | 2.51                     | 0.45              |
| 1:AS:1852:C:H2'    | 1:AS:1853:C:C6     | 2.51                     | 0.45              |
| 1:AS:2367:C:H2'    | 1:AS:2368:A:C8     | 2.51                     | 0.45              |
| 1:AS:2385:C:H1'    | 1:AS:2790:U:C2     | 2.52                     | 0.45              |
| 1:AS:2401:U:H2'    | 1:AS:2402:A:C8     | 2.51                     | 0.45              |
| 1:AS:2484:U:H2'    | 1:AS:2485:U:H6     | 1.80                     | 0.45              |
| 1:AS:2514:G:N7     | 1:AS:2515:G:N1     | 2.64                     | 0.45              |
| 1:AS:2627:U:H4'    | 1:AS:2628:A:O4'    | 2.17                     | 0.45              |
| 1:AS:3270:A:H2'    | 1:AS:3271:U:O4'    | 2.17                     | 0.45              |
| 6:AY:65:SER:HA     | 6:AY:76:PRO:HA     | 1.97                     | 0.45              |
| 13:BF:109:HIS:CD2  | 13:BF:122:ILE:HD12 | 2.51                     | 0.45              |
| 16:BI:123:GLN:HG3  | 16:BI:128:LYS:HG2  | 1.98                     | 0.45              |
| 18:BK:123:PRO:O    | 18:BK:143:PRO:HG2  | 2.17                     | 0.45              |
| 18:BK:165:GLN:OE1  | 18:BK:165:GLN:N    | 2.50                     | 0.45              |
| 21:BN:164:GLN:HG2  | 21:BN:166:THR:H    | 1.82                     | 0.45              |
| 46:CM:565:A:H1'    | 77:DR:14:VAL:HG23  | 1.98                     | 0.45              |
| 46:CM:761:G:N2     | 46:CM:769:U:H1'    | 2.32                     | 0.45              |
| 46:CM:917:U:O2     | 73:DN:32:LYS:HE3   | 2.16                     | 0.45              |
| 46:CM:1233:C:C2    | 46:CM:1234:U:C5    | 3.05                     | 0.45              |
| 48:CO:64:ARG:O     | 48:CO:88:VAL:HG12  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:CT:84:TYR:CE1  | 53:CT:93:LYS:HB2   | 2.51                     | 0.45              |
| 54:CU:122:LEU:CD1 | 54:CU:169:TYR:CD1  | 2.92                     | 0.45              |
| 56:CW:63:ASP:OD1  | 56:CW:64:GLU:N     | 2.49                     | 0.45              |
| 59:CZ:58:GLN:HB3  | 59:CZ:87:PRO:HG2   | 1.99                     | 0.45              |
| 62:DC:34:THR:HB   | 62:DC:45:PHE:CD2   | 2.52                     | 0.45              |
| 62:DC:64:ARG:HH22 | 62:DC:91:GLY:HA3   | 1.81                     | 0.45              |
| 70:DK:100:ASP:OD2 | 70:DK:142:LYS:NZ   | 2.38                     | 0.45              |
| 1:1:95:G:H5'      | 14:t:15:ARG:CZ     | 2.47                     | 0.45              |
| 1:1:538:G:C6      | 1:1:548:G:C6       | 3.04                     | 0.45              |
| 1:1:1651:G:H5''   | 35:AH:58:ARG:NH1   | 2.32                     | 0.45              |
| 1:1:2183:U:O2'    | 1:1:2184:G:OP1     | 2.29                     | 0.45              |
| 1:1:2455:G:H2'    | 1:1:2456:C:C5      | 2.52                     | 0.45              |
| 1:1:2685:U:O2'    | 43:AP:8:ARG:NE     | 2.50                     | 0.45              |
| 1:1:2972:A:H2'    | 1:1:2973:U:C6      | 2.52                     | 0.45              |
| 1:1:3138:U:C2     | 1:1:3139:U:C5      | 3.05                     | 0.45              |
| 5:k:293:ASN:HB2   | 5:k:304:THR:HA     | 1.99                     | 0.45              |
| 8:n:45:ARG:NH1    | 18:x:178:SER:HB3   | 2.25                     | 0.45              |
| 10:p:122:THR:C    | 10:p:124:LYS:H     | 2.24                     | 0.45              |
| 17:w:189:SER:O    | 17:w:193:GLN:HG2   | 2.16                     | 0.45              |
| 19:y:96:PHE:CD1   | 19:y:97:PRO:HD2    | 2.52                     | 0.45              |
| 25:7:85:ALA:HA    | 25:7:89:LEU:HD13   | 1.97                     | 0.45              |
| 31:AD:9:GLN:O     | 31:AD:10:GLU:C     | 2.60                     | 0.45              |
| 46:B:383:A:H2'    | 46:B:384:G:C8      | 2.52                     | 0.45              |
| 46:B:654:G:H3'    | 46:B:655:U:H6      | 1.80                     | 0.45              |
| 46:B:1183:G:O4'   | 67:W:72:GLY:HA3    | 2.16                     | 0.45              |
| 46:B:1313:G:H5'   | 50:F:160:HIS:HB2   | 1.98                     | 0.45              |
| 46:B:1649:G:H2'   | 46:B:1650:G:H8     | 1.82                     | 0.45              |
| 54:J:11:THR:HG23  | 54:J:14:GLU:H      | 1.82                     | 0.45              |
| 54:J:162:LEU:O    | 54:J:166:GLN:HG3   | 2.16                     | 0.45              |
| 1:AS:487:C:H3'    | 1:AS:488:G:C8      | 2.52                     | 0.45              |
| 1:AS:716:G:O2'    | 1:AS:717:A:OP1     | 2.30                     | 0.45              |
| 1:AS:1417:G:H2'   | 1:AS:1418:G:C8     | 2.51                     | 0.45              |
| 1:AS:2481:G:H2'   | 1:AS:2482:U:C6     | 2.52                     | 0.45              |
| 1:AS:2650:A:C8    | 45:CL:56:SER:HB2   | 2.52                     | 0.45              |
| 10:BC:92:PHE:O    | 10:BC:96:ASN:ND2   | 2.48                     | 0.45              |
| 10:BC:171:CYS:HB3 | 10:BC:176:VAL:O    | 2.17                     | 0.45              |
| 11:BD:135:GLU:O   | 11:BD:144:LEU:HD12 | 2.17                     | 0.45              |
| 11:BD:165:CYS:HB3 | 11:BD:178:GLY:HA2  | 1.98                     | 0.45              |
| 14:BG:46:ILE:O    | 14:BG:47:ALA:C     | 2.60                     | 0.45              |
| 14:BG:122:LYS:HD2 | 14:BG:147:PHE:HZ   | 1.81                     | 0.45              |
| 16:BI:36:ILE:HG12 | 16:BI:64:ILE:HG13  | 1.99                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:BI:68:ARG:HH11  | 16:BI:125:SER:HA  | 1.80                     | 0.45              |
| 23:BP:101:VAL:HG13 | 23:BP:107:LYS:HG2 | 1.99                     | 0.45              |
| 26:BS:74:LYS:HA    | 26:BS:77:GLU:HG2  | 1.98                     | 0.45              |
| 44:CK:47:VAL:HA    | 44:CK:56:ASN:O    | 2.15                     | 0.45              |
| 46:CM:690:C:H4'    | 46:CM:691:U:OP1   | 2.16                     | 0.45              |
| 55:CV:65:PHE:HZ    | 55:CV:78:ILE:HD11 | 1.79                     | 0.45              |
| 57:CX:46:LEU:HD23  | 57:CX:66:TYR:CG   | 2.51                     | 0.45              |
| 62:DC:68:GLU:CD    | 62:DC:68:GLU:H    | 2.24                     | 0.45              |
| 64:DE:5:ARG:O      | 64:DE:10:LYS:HE2  | 2.17                     | 0.45              |
| 64:DE:72:LYS:HA    | 64:DE:72:LYS:HD2  | 1.72                     | 0.45              |
| 75:DP:9:LEU:C      | 75:DP:33:LEU:HD23 | 2.42                     | 0.45              |
| 79:DT:21:THR:O     | 79:DT:288:SER:HB2 | 2.15                     | 0.45              |
| 79:DT:177:SER:C    | 79:DT:186:ASN:HB2 | 2.42                     | 0.45              |
| 81:P0:44:ALA:C     | 81:P0:45:LEU:HD23 | 2.42                     | 0.45              |
| 1:1:179:C:H2'      | 1:1:180:U:H6      | 1.81                     | 0.45              |
| 1:1:548:G:H2'      | 1:1:549:U:C6      | 2.51                     | 0.45              |
| 1:1:861:U:C2       | 1:1:862:A:C8      | 3.05                     | 0.45              |
| 1:1:1247:A:C2      | 82:12:139:VAL:HA  | 2.52                     | 0.45              |
| 1:1:1325:U:O3'     | 34:AG:19:SER:OG   | 2.34                     | 0.45              |
| 1:1:1652:A:H8      | 1:1:1652:A:OP1    | 1.99                     | 0.45              |
| 1:1:1814:U:O2'     | 1:1:1815:U:O5'    | 2.33                     | 0.45              |
| 1:1:2958:U:C2      | 1:1:2959:A:C8     | 3.05                     | 0.45              |
| 1:1:3068:C:H2'     | 1:1:3069:U:C6     | 2.52                     | 0.45              |
| 3:4:26:U:H2'       | 3:4:27:U:C6       | 2.52                     | 0.45              |
| 7:m:40:HIS:CE1     | 7:m:42:ALA:HB3    | 2.51                     | 0.45              |
| 9:o:71:ASN:O       | 22:2:143:THR:OG1  | 2.31                     | 0.45              |
| 46:B:303:C:H2'     | 46:B:304:U:C6     | 2.51                     | 0.45              |
| 46:B:458:A:O2'     | 51:G:27:TYR:OH    | 2.11                     | 0.45              |
| 46:B:553:A:H2'     | 46:B:554:A:C8     | 2.52                     | 0.45              |
| 46:B:565:A:N3      | 77:g:14:VAL:HG21  | 2.32                     | 0.45              |
| 46:B:622:G:H2'     | 46:B:623:C:C6     | 2.51                     | 0.45              |
| 46:B:649:G:H3'     | 46:B:650:G:H8     | 1.81                     | 0.45              |
| 46:B:1149:G:H2'    | 46:B:1150:G:H8    | 1.81                     | 0.45              |
| 48:D:28:ASP:OD2    | 48:D:50:ARG:HG3   | 2.17                     | 0.45              |
| 48:D:160:LYS:HA    | 48:D:160:LYS:HD2  | 1.87                     | 0.45              |
| 50:F:9:LYS:HG2     | 67:W:62:LEU:HD11  | 1.98                     | 0.45              |
| 50:F:30:LEU:HD22   | 50:F:33:GLN:OE1   | 2.17                     | 0.45              |
| 59:O:28:LEU:HA     | 59:O:31:VAL:HG22  | 1.98                     | 0.45              |
| 59:O:40:GLY:O      | 59:O:41:LEU:HB3   | 2.17                     | 0.45              |
| 61:Q:79:ARG:HB3    | 61:Q:113:VAL:HG23 | 1.99                     | 0.45              |
| 63:S:22:LYS:HG2    | 63:S:23:ALA:H     | 1.82                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 67:W:56:ARG:HG3   | 67:W:88:ARG:NH1    | 2.31                     | 0.45              |
| 79:AR:84:ALA:HA   | 79:AR:90:LEU:HD23  | 1.99                     | 0.45              |
| 1:AS:481:G:P      | 1:AS:481:G:O4'     | 2.75                     | 0.45              |
| 1:AS:547:U:H2'    | 1:AS:548:G:C8      | 2.51                     | 0.45              |
| 1:AS:777:G:OP1    | 19:BL:151:ARG:HD2  | 2.17                     | 0.45              |
| 1:AS:1428:C:O2'   | 1:AS:1430:G:OP2    | 2.33                     | 0.45              |
| 1:AS:3321:G:C6    | 1:AS:3322:U:C4     | 3.05                     | 0.45              |
| 3:AU:95:G:OP2     | 38:CE:72:ARG:NE    | 2.49                     | 0.45              |
| 46:CM:154:A:H2'   | 46:CM:155:A:O4'    | 2.17                     | 0.45              |
| 46:CM:295:U:H2'   | 46:CM:296:C:C6     | 2.52                     | 0.45              |
| 46:CM:806:A:OP1   | 46:CM:806:A:H3'    | 2.17                     | 0.45              |
| 46:CM:1052:G:H5'' | 48:CO:150:ILE:HG12 | 1.97                     | 0.45              |
| 48:CO:24:PHE:CE2  | 61:DB:65:LYS:HE3   | 2.49                     | 0.45              |
| 53:CT:126:ASP:OD1 | 53:CT:127:THR:N    | 2.50                     | 0.45              |
| 54:CU:102:ALA:O   | 54:CU:103:ARG:HD3  | 2.16                     | 0.45              |
| 55:CV:17:LYS:HD3  | 55:CV:17:LYS:HA    | 1.77                     | 0.45              |
| 59:CZ:62:LEU:HD22 | 59:CZ:71:ILE:CG2   | 2.47                     | 0.45              |
| 66:DG:108:LEU:HA  | 66:DG:111:ILE:HG22 | 1.99                     | 0.45              |
| 1:1:155:A:OP2     | 37:AJ:24:LYS:HB3   | 2.17                     | 0.45              |
| 1:1:174:C:H2'     | 1:1:175:G:O4'      | 2.17                     | 0.45              |
| 1:1:242:C:O2'     | 1:1:243:G:H8       | 2.00                     | 0.45              |
| 1:1:699:G:H2'     | 1:1:700:C:H6       | 1.82                     | 0.45              |
| 1:1:716:G:OP1     | 29:AB:117:ARG:NH2  | 2.50                     | 0.45              |
| 1:1:777:G:OP1     | 19:y:151:ARG:HD2   | 2.17                     | 0.45              |
| 1:1:814:C:H2'     | 1:1:815:U:O4'      | 2.17                     | 0.45              |
| 1:1:859:C:H2'     | 1:1:860:G:O4'      | 2.17                     | 0.45              |
| 1:1:1153:G:H5''   | 9:o:217:PHE:CE2    | 2.52                     | 0.45              |
| 1:1:1593:C:H4'    | 35:AH:26:PRO:HD2   | 1.98                     | 0.45              |
| 1:1:1789:C:H2'    | 4:j:184:ARG:HH22   | 1.81                     | 0.45              |
| 2:3:16:U:H2'      | 2:3:17:A:H8        | 1.80                     | 0.45              |
| 4:j:32:LEU:HD13   | 4:j:163:ARG:HD3    | 1.98                     | 0.45              |
| 12:r:86:HIS:HD2   | 12:r:139:ARG:HD3   | 1.82                     | 0.45              |
| 12:r:170:LYS:NZ   | 12:r:177:ASN:OD1   | 2.50                     | 0.45              |
| 19:y:150:VAL:HA   | 19:y:153:PHE:CD2   | 2.52                     | 0.45              |
| 31:AD:12:ILE:O    | 31:AD:13:ASN:C     | 2.60                     | 0.45              |
| 33:AF:98:ALA:HB3  | 33:AF:101:VAL:HG23 | 1.98                     | 0.45              |
| 34:AG:20:LYS:HE2  | 34:AG:20:LYS:HB2   | 1.68                     | 0.45              |
| 46:B:46:A:N1      | 46:B:430:G:O2'     | 2.42                     | 0.45              |
| 46:B:189:G:H1'    | 46:B:193:G:C2      | 2.51                     | 0.45              |
| 46:B:983:A:N6     | 46:B:989:U:OP2     | 2.50                     | 0.45              |
| 46:B:985:C:H6     | 46:B:988:A:C8      | 2.35                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:1011:A:N3    | 46:B:1777:A:O2'    | 2.44                     | 0.45              |
| 46:B:1336:G:OP1   | 63:S:20:HIS:NE2    | 2.50                     | 0.45              |
| 46:B:1354:U:H2'   | 46:B:1355:A:H8     | 1.82                     | 0.45              |
| 46:B:1593:C:H2'   | 46:B:1594:G:C8     | 2.52                     | 0.45              |
| 46:B:1776:G:OP2   | 61:Q:127:ARG:NH2   | 2.40                     | 0.45              |
| 47:C:200:ASP:HB2  | 64:T:85:VAL:HG23   | 1.98                     | 0.45              |
| 54:J:149:LEU:HA   | 54:J:180:GLU:O     | 2.17                     | 0.45              |
| 57:M:4:PRO:HG2    | 57:M:7:ASP:HB2     | 1.99                     | 0.45              |
| 59:O:33:ARG:O     | 59:O:33:ARG:HD3    | 2.17                     | 0.45              |
| 59:O:99:GLU:OE2   | 59:O:111:ASN:HB3   | 2.17                     | 0.45              |
| 63:S:22:LYS:HG2   | 63:S:23:ALA:N      | 2.32                     | 0.45              |
| 75:e:12:VAL:CG2   | 75:e:52:ASP:H      | 2.29                     | 0.45              |
| 79:AR:50:GLY:N    | 79:AR:55:TYR:HA    | 2.29                     | 0.45              |
| 79:AR:121:ARG:HA  | 79:AR:137:THR:OG1  | 2.17                     | 0.45              |
| 1:AS:4:G:C6       | 3:AU:155:G:O6      | 2.70                     | 0.45              |
| 1:AS:779:A:H5''   | 1:AS:780:A:H5''    | 1.99                     | 0.45              |
| 1:AS:872:A:H5''   | 1:AS:1886:U:H5''   | 1.99                     | 0.45              |
| 1:AS:2713:C:HO2'  | 43:CJ:20:HIS:CE1   | 2.28                     | 0.45              |
| 9:BB:130:PRO:HG2  | 9:BB:131:TYR:CE2   | 2.51                     | 0.45              |
| 10:BC:227:TYR:CE2 | 10:BC:231:ARG:HD2  | 2.52                     | 0.45              |
| 11:BD:47:LYS:HZ3  | 15:BH:3:SER:HA     | 1.81                     | 0.45              |
| 21:BN:154:HIS:HA  | 21:BN:170:THR:HB   | 1.98                     | 0.45              |
| 23:BP:35:LYS:O    | 23:BP:39:GLU:HB2   | 2.17                     | 0.45              |
| 25:BR:93:ARG:NH1  | 53:CT:156:PHE:HA   | 2.32                     | 0.45              |
| 36:CC:63:ARG:O    | 36:CC:67:ARG:HB2   | 2.17                     | 0.45              |
| 46:CM:339:A:H2'   | 46:CM:340:C:C6     | 2.52                     | 0.45              |
| 46:CM:520:U:H2'   | 46:CM:521:G:O4'    | 2.17                     | 0.45              |
| 46:CM:521:G:N2    | 46:CM:526:U:OP2    | 2.41                     | 0.45              |
| 46:CM:1032:G:H2'  | 46:CM:1033:U:H6    | 1.82                     | 0.45              |
| 46:CM:1478:A:O2'  | 46:CM:1479:A:O4'   | 2.28                     | 0.45              |
| 46:CM:1584:A:C8   | 76:DQ:14:PHE:CD1   | 3.05                     | 0.45              |
| 48:CO:30:PHE:HB2  | 48:CO:96:LEU:CD1   | 2.47                     | 0.45              |
| 61:DB:11:VAL:HG12 | 61:DB:13:ARG:HG3   | 1.99                     | 0.45              |
| 75:DP:30:VAL:HG22 | 75:DP:40:ILE:O     | 2.16                     | 0.45              |
| 79:DT:110:ASP:O   | 79:DT:112:LEU:HD13 | 2.17                     | 0.45              |
| 1:1:294:U:OP2     | 16:v:15:GLN:NE2    | 2.39                     | 0.45              |
| 1:1:605:U:C2      | 8:n:25:ARG:NH1     | 2.85                     | 0.45              |
| 1:1:638:U:OP2     | 33:AF:39:ILE:HG12  | 2.17                     | 0.45              |
| 1:1:844:A:C5      | 1:1:845:C:H1'      | 2.51                     | 0.45              |
| 1:1:1642:G:H1'    | 1:1:1805:A:H61     | 1.82                     | 0.45              |
| 1:1:1655:U:H2'    | 1:1:1656:C:H6      | 1.80                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:l:2145:A:H2'     | 1:l:2146:A:C8     | 2.52                     | 0.45              |
| 6:l:38:SER:HG      | 6:l:42:ARG:HH21   | 1.62                     | 0.45              |
| 8:n:39:LEU:HB3     | 8:n:83:VAL:HG13   | 1.99                     | 0.45              |
| 11:q:8:GLN:HB3     | 11:q:72:LYS:HD2   | 1.98                     | 0.45              |
| 14:t:173:ARG:HA    | 14:t:173:ARG:HD2  | 1.78                     | 0.45              |
| 23:5:38:VAL:HA     | 23:5:56:ILE:HD12  | 1.99                     | 0.45              |
| 26:8:105:VAL:HG23  | 26:8:130:TYR:CG   | 2.52                     | 0.45              |
| 36:AI:70:TYR:HA    | 36:AI:73:LYS:HG3  | 1.98                     | 0.45              |
| 40:AM:23:LEU:HD12  | 40:AM:24:PRO:HD2  | 1.98                     | 0.45              |
| 46:B:36:C:H2'      | 46:B:37:U:H6      | 1.82                     | 0.45              |
| 46:B:219:A:H3'     | 46:B:818:U:O2     | 2.16                     | 0.45              |
| 46:B:850:A:OP1     | 69:Y:28:ARG:NH2   | 2.43                     | 0.45              |
| 46:B:963:A:H2'     | 46:B:964:A:O4'    | 2.16                     | 0.45              |
| 46:B:1445:C:H2'    | 65:U:138:THR:OG1  | 2.17                     | 0.45              |
| 46:B:1634:U:H2'    | 46:B:1635:A:C8    | 2.51                     | 0.45              |
| 46:B:1740:A:H2'    | 46:B:1741:A:C8    | 2.52                     | 0.45              |
| 46:B:1753:A:H61    | 73:c:80:HIS:HA    | 1.81                     | 0.45              |
| 51:G:197:HIS:CE1   | 51:G:199:GLU:HB2  | 2.52                     | 0.45              |
| 53:I:20:ASP:HB3    | 53:I:23:LYS:HE3   | 1.99                     | 0.45              |
| 1:AS:870:U:N3      | 1:AS:2950:U:OP1   | 2.42                     | 0.45              |
| 1:AS:1153:G:H2'    | 1:AS:1154:A:O4'   | 2.17                     | 0.45              |
| 1:AS:1199:A:H1'    | 1:AS:2828:G:O5'   | 2.17                     | 0.45              |
| 1:AS:1896:A:O2'    | 1:AS:1902:G:N7    | 2.40                     | 0.45              |
| 1:AS:2242:U:H2'    | 1:AS:2243:C:H6    | 1.81                     | 0.45              |
| 1:AS:2391:A:H2'    | 1:AS:2392:G:C8    | 2.51                     | 0.45              |
| 1:AS:2411:U:OP2    | 1:AS:2412:U:O2'   | 2.23                     | 0.45              |
| 1:AS:3208:A:H62    | 17:BJ:161:ARG:HB2 | 1.82                     | 0.45              |
| 1:AS:3319:U:H3     | 55:CV:107:THR:HG1 | 1.65                     | 0.45              |
| 1:AS:3340:A:H5''   | 32:BY:17:LYS:HD3  | 1.99                     | 0.45              |
| 83:AS:3401:3K5:H27 | 43:CJ:43:TYR:CD2  | 2.51                     | 0.45              |
| 3:AU:56:G:H5''     | 38:CE:68:LYS:HZ3  | 1.81                     | 0.45              |
| 3:AU:104:A:C8      | 3:AU:105:A:C8     | 3.05                     | 0.45              |
| 7:AZ:160:PHE:HB3   | 7:AZ:180:PHE:CE1  | 2.52                     | 0.45              |
| 9:BB:118:THR:H     | 9:BB:121:THR:HG1  | 1.62                     | 0.45              |
| 14:BG:104:LYS:HE3  | 14:BG:104:LYS:HB2 | 1.73                     | 0.45              |
| 14:BG:184:ILE:HD12 | 14:BG:187:LYS:HD3 | 1.99                     | 0.45              |
| 20:BM:160:GLU:OE2  | 20:BM:163:ARG:HB3 | 2.17                     | 0.45              |
| 28:BU:101:LEU:O    | 28:BU:107:ARG:NH1 | 2.50                     | 0.45              |
| 46:CM:217:A:C5'    | 46:CM:816:U:HO2'  | 2.26                     | 0.45              |
| 46:CM:303:C:H2'    | 46:CM:304:U:C6    | 2.51                     | 0.45              |
| 46:CM:542:A:H4'    | 77:DR:28:LYS:NZ   | 2.32                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:CM:1425:C:H2'  | 46:CM:1426:C:H6    | 1.82                     | 0.45              |
| 46:CM:1500:G:H1'  | 46:CM:1505:C:O2    | 2.16                     | 0.45              |
| 48:CO:178:ASN:OD1 | 48:CO:178:ASN:C    | 2.60                     | 0.45              |
| 59:CZ:62:LEU:HD21 | 59:CZ:75:VAL:HG21  | 1.98                     | 0.45              |
| 63:DD:68:VAL:HG11 | 63:DD:80:ILE:HD11  | 1.99                     | 0.45              |
| 73:DN:3:LYS:NZ    | 73:DN:6:ALA:HA     | 2.32                     | 0.45              |
| 1:1:130:U:H2'     | 1:1:131:C:H6       | 1.83                     | 0.44              |
| 1:1:142:G:H4'     | 3:4:145:U:OP1      | 2.17                     | 0.44              |
| 1:1:496:A:C4'     | 8:n:27:GLN:HG3     | 2.41                     | 0.44              |
| 1:1:716:G:O2'     | 1:1:717:A:OP1      | 2.30                     | 0.44              |
| 1:1:943:G:H2'     | 1:1:944:C:C6       | 2.52                     | 0.44              |
| 1:1:1303:G:H4'    | 1:1:1304:A:O5'     | 2.17                     | 0.44              |
| 1:1:1312:C:OP2    | 17:w:134:ARG:HG3   | 2.18                     | 0.44              |
| 1:1:1932:A:H5''   | 46:B:1655:G:H5'    | 1.97                     | 0.44              |
| 1:1:2736:C:O2     | 83:1:3401:3K5:H35  | 2.17                     | 0.44              |
| 4:j:186:PHE:HB2   | 4:j:196:TRP:CZ3    | 2.53                     | 0.44              |
| 12:r:38:ARG:HG2   | 12:r:41:ALA:HB2    | 1.99                     | 0.44              |
| 12:r:189:GLU:CD   | 12:r:200:LEU:HB3   | 2.42                     | 0.44              |
| 16:v:119:TYR:OH   | 16:v:131:GLU:OE1   | 2.27                     | 0.44              |
| 23:5:37:LEU:HB3   | 23:5:56:ILE:HD13   | 1.99                     | 0.44              |
| 46:B:17:C:H4'     | 46:B:1094:G:C8     | 2.52                     | 0.44              |
| 46:B:734:U:C4     | 46:B:785:G:C6      | 3.05                     | 0.44              |
| 46:B:1636:C:H2'   | 46:B:1637:U:C6     | 2.52                     | 0.44              |
| 50:F:176:VAL:HB   | 50:F:183:LEU:HB2   | 1.98                     | 0.44              |
| 52:H:99:MET:O     | 52:H:103:ASN:HB2   | 2.17                     | 0.44              |
| 58:N:73:GLY:HA3   | 58:N:86:ILE:HD12   | 1.98                     | 0.44              |
| 68:X:4:ASP:OD1    | 68:X:5:LYS:N       | 2.49                     | 0.44              |
| 1:AS:1637:U:O2'   | 1:AS:1638:A:H3'    | 2.17                     | 0.44              |
| 1:AS:1725:A:C6    | 31:BX:51:PRO:HD3   | 2.51                     | 0.44              |
| 1:AS:2557:G:C6    | 26:BS:24:LEU:HD11  | 2.53                     | 0.44              |
| 1:AS:2996:A:H5''  | 11:BD:96:HIS:CE1   | 2.52                     | 0.44              |
| 1:AS:3019:U:OP1   | 5:AX:222:LYS:N     | 2.50                     | 0.44              |
| 1:AS:3123:U:H4'   | 1:AS:3259:A:H1'    | 1.99                     | 0.44              |
| 10:BC:62:GLN:HA   | 10:BC:65:ILE:HD13  | 1.99                     | 0.44              |
| 19:BL:158:HIS:NE2 | 19:BL:186:VAL:HG12 | 2.32                     | 0.44              |
| 35:CB:55:SER:OG   | 35:CB:69:HIS:HB3   | 2.16                     | 0.44              |
| 46:CM:289:G:H2'   | 46:CM:290:U:C5     | 2.51                     | 0.44              |
| 46:CM:327:G:H5'   | 55:CV:99:SER:HB3   | 1.99                     | 0.44              |
| 46:CM:397:A:H1'   | 46:CM:399:A:O4'    | 2.17                     | 0.44              |
| 46:CM:415:A:H5'   | 46:CM:416:G:C5     | 2.52                     | 0.44              |
| 46:CM:904:A:H2'   | 46:CM:905:C:H6     | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:CM:994:U:OP2   | 61:DB:124:LYS:NZ  | 2.34                     | 0.44              |
| 46:CM:1516:C:H2'  | 46:CM:1517:C:H6   | 1.82                     | 0.44              |
| 46:CM:1784:A:H2   | 73:DN:98:PRO:HG3  | 1.82                     | 0.44              |
| 48:CO:144:LYS:HE2 | 48:CO:206:PRO:HB3 | 1.99                     | 0.44              |
| 54:CU:126:VAL:O   | 54:CU:127:PHE:C   | 2.60                     | 0.44              |
| 56:CW:81:VAL:HG21 | 56:CW:91:MET:HE2  | 1.98                     | 0.44              |
| 61:DB:76:ILE:HD13 | 61:DB:97:LEU:CD1  | 2.46                     | 0.44              |
| 61:DB:117:PRO:HB2 | 61:DB:120:SER:HB3 | 1.99                     | 0.44              |
| 66:DG:86:ARG:HD3  | 66:DG:90:PRO:O    | 2.17                     | 0.44              |
| 69:DJ:77:PRO:HD3  | 70:DK:7:ARG:O     | 2.17                     | 0.44              |
| 79:DT:170:SER:HB3 | 79:DT:172:ASP:OD1 | 2.16                     | 0.44              |
| 81:P0:16:ARG:HD2  | 81:P0:66:PHE:CZ   | 2.51                     | 0.44              |
| 1:1:6:C:H2'       | 1:1:7:C:C6        | 2.53                     | 0.44              |
| 1:1:62:A:H5''     | 16:v:174:ILE:HG21 | 2.00                     | 0.44              |
| 1:1:209:C:C2      | 6:l:218:LYS:HD3   | 2.53                     | 0.44              |
| 1:1:361:A:N1      | 1:1:923:C:O2'     | 2.50                     | 0.44              |
| 1:1:1275:C:H2'    | 1:1:1276:C:C6     | 2.52                     | 0.44              |
| 1:1:1556:G:O2'    | 1:1:1557:U:H5'    | 2.17                     | 0.44              |
| 1:1:1652:A:H4'    | 1:1:1653:C:O4'    | 2.18                     | 0.44              |
| 6:l:360:VAL:HA    | 21:0:26:ARG:HH12  | 1.81                     | 0.44              |
| 20:z:168:ALA:O    | 20:z:172:ARG:HG3  | 2.18                     | 0.44              |
| 27:9:37:LYS:HZ3   | 27:9:40:ARG:HH11  | 1.65                     | 0.44              |
| 31:AD:11:ASN:O    | 31:AD:12:ILE:C    | 2.60                     | 0.44              |
| 36:AI:7:PHE:CE1   | 36:AI:8:GLU:HG3   | 2.52                     | 0.44              |
| 42:AO:1:MET:HB3   | 46:B:1629:G:H5'   | 1.99                     | 0.44              |
| 46:B:149:G:N2     | 53:I:13:GLN:OE1   | 2.31                     | 0.44              |
| 46:B:839:U:O4     | 46:B:840:A:N6     | 2.50                     | 0.44              |
| 46:B:975:C:H2'    | 46:B:976:G:O4'    | 2.17                     | 0.44              |
| 46:B:1204:A:O2'   | 57:M:48:SER:HA    | 2.16                     | 0.44              |
| 46:B:1435:U:H2'   | 46:B:1436:U:H6    | 1.83                     | 0.44              |
| 46:B:1668:A:H2'   | 46:B:1669:U:H5'   | 1.98                     | 0.44              |
| 47:C:10:THR:HG23  | 47:C:13:ASP:H     | 1.81                     | 0.44              |
| 70:Z:63:GLN:OE1   | 70:Z:64:PRO:HA    | 2.17                     | 0.44              |
| 71:a:41:ARG:NH2   | 71:a:94:TYR:HB3   | 2.33                     | 0.44              |
| 72:b:54:VAL:HG13  | 72:b:60:VAL:HG11  | 1.99                     | 0.44              |
| 1:AS:952:U:H2'    | 1:AS:953:C:C6     | 2.53                     | 0.44              |
| 1:AS:2127:A:O3'   | 4:AW:179:LEU:HB2  | 2.17                     | 0.44              |
| 1:AS:2138:G:H2'   | 1:AS:2139:G:C8    | 2.51                     | 0.44              |
| 1:AS:2854:U:H2'   | 1:AS:2855:U:H6    | 1.83                     | 0.44              |
| 1:AS:2915:G:H2'   | 1:AS:2916:U:O4'   | 2.17                     | 0.44              |
| 1:AS:3264:C:H2'   | 1:AS:3265:U:C6    | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:BI:193:LYS:HE2 | 16:BI:193:LYS:HB3 | 1.79                     | 0.44              |
| 19:BL:40:THR:C    | 19:BL:42:ALA:H    | 2.24                     | 0.44              |
| 45:CL:88:PHE:HB3  | 45:CL:91:HIS:ND1  | 2.31                     | 0.44              |
| 46:CM:502:U:H2'   | 46:CM:503:A:H8    | 1.81                     | 0.44              |
| 46:CM:769:U:O2'   | 46:CM:770:C:OP2   | 2.33                     | 0.44              |
| 46:CM:811:U:H2'   | 46:CM:812:C:H6    | 1.81                     | 0.44              |
| 46:CM:825:U:C4    | 46:CM:826:U:C4    | 3.05                     | 0.44              |
| 46:CM:1032:G:H2'  | 46:CM:1033:U:C6   | 2.52                     | 0.44              |
| 46:CM:1351:U:H2'  | 46:CM:1352:G:O4'  | 2.17                     | 0.44              |
| 46:CM:1437:C:OP1  | 76:DQ:12:ARG:NH1  | 2.47                     | 0.44              |
| 46:CM:1529:G:H5'' | 66:DG:87:GLY:CA   | 2.47                     | 0.44              |
| 46:CM:1577:G:OP1  | 66:DG:91:HIS:HB2  | 2.17                     | 0.44              |
| 48:CO:69:CYS:HB3  | 48:CO:72:ASP:OD2  | 2.17                     | 0.44              |
| 49:CP:225:TRP:O   | 68:DI:16:LYS:NZ   | 2.50                     | 0.44              |
| 53:CT:149:LYS:HB3 | 53:CT:149:LYS:HE2 | 1.64                     | 0.44              |
| 54:CU:40:LYS:NZ   | 54:CU:58:VAL:C    | 2.75                     | 0.44              |
| 54:CU:51:LYS:HB2  | 54:CU:83:ASP:O    | 2.16                     | 0.44              |
| 54:CU:68:LYS:O    | 54:CU:72:ARG:NH2  | 2.50                     | 0.44              |
| 54:CU:70:GLN:OE1  | 54:CU:127:PHE:HB2 | 2.18                     | 0.44              |
| 57:CX:50:THR:HG21 | 57:CX:57:THR:HG22 | 1.98                     | 0.44              |
| 64:DE:61:ILE:HD11 | 64:DE:69:ILE:CD1  | 2.47                     | 0.44              |
| 78:DS:177:MET:HE1 | 78:DS:180:ARG:NH2 | 2.33                     | 0.44              |
| 79:DT:201:LEU:N   | 79:DT:201:LEU:CD2 | 2.75                     | 0.44              |
| 81:P0:49:ALA:HB1  | 81:P0:88:PHE:O    | 2.17                     | 0.44              |
| 1:1:171:G:H2'     | 1:1:172:C:C6      | 2.52                     | 0.44              |
| 1:1:661:C:H2'     | 1:1:662:U:C6      | 2.52                     | 0.44              |
| 1:1:1396:U:H2'    | 1:1:1397:G:O4'    | 2.17                     | 0.44              |
| 1:1:1424:A:OP2    | 29:AB:2:PRO:HA    | 2.17                     | 0.44              |
| 1:1:2686:G:OP2    | 43:AP:10:THR:HG22 | 2.17                     | 0.44              |
| 1:1:3260:A:H2'    | 1:1:3261:A:C8     | 2.52                     | 0.44              |
| 2:3:97:A:H2'      | 2:3:98:C:C6       | 2.52                     | 0.44              |
| 3:4:57:C:OP2      | 38:AK:68:LYS:NZ   | 2.49                     | 0.44              |
| 3:4:126:A:O2'     | 3:4:128:U:OP2     | 2.23                     | 0.44              |
| 9:o:82:VAL:HG21   | 9:o:134:TYR:HD2   | 1.82                     | 0.44              |
| 13:s:132:GLY:HA2  | 13:s:154:THR:HG21 | 1.99                     | 0.44              |
| 16:v:67:ARG:HG2   | 16:v:127:TYR:CE1  | 2.53                     | 0.44              |
| 18:x:23:ARG:O     | 18:x:86:LYS:NZ    | 2.43                     | 0.44              |
| 39:AL:46:ARG:HD3  | 39:AL:47:GLY:O    | 2.18                     | 0.44              |
| 45:i:65:LYS:O     | 45:i:66:ASN:ND2   | 2.36                     | 0.44              |
| 46:B:4:C:H4'      | 49:E:176:SER:HB3  | 1.99                     | 0.44              |
| 46:B:25:C:H4'     | 46:B:26:A:O5'     | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:79:C:H1'     | 53:I:174:LYS:HB2  | 1.98                     | 0.44              |
| 46:B:400:C:OP1    | 51:G:3:ARG:NH1    | 2.50                     | 0.44              |
| 46:B:627:U:C2     | 46:B:628:A:C8     | 3.06                     | 0.44              |
| 46:B:1160:U:H3    | 46:B:1450:G:H1    | 1.65                     | 0.44              |
| 46:B:1168:A:O2'   | 46:B:1169:A:OP1   | 2.35                     | 0.44              |
| 46:B:1216:U:OP1   | 46:B:1244:U:H1'   | 2.17                     | 0.44              |
| 46:B:1235:U:O2'   | 78:h:177:MET:HB3  | 2.18                     | 0.44              |
| 46:B:1248:G:H2'   | 46:B:1249:G:O4'   | 2.16                     | 0.44              |
| 46:B:1425:C:H2'   | 46:B:1426:C:H6    | 1.82                     | 0.44              |
| 46:B:1716:C:H2'   | 46:B:1717:A:O4'   | 2.16                     | 0.44              |
| 48:D:131:ASP:OD1  | 48:D:131:ASP:N    | 2.47                     | 0.44              |
| 51:G:68:GLN:NE2   | 51:G:76:VAL:HG11  | 2.33                     | 0.44              |
| 78:h:147:TYR:HD2  | 78:h:173:PHE:CD2  | 2.36                     | 0.44              |
| 1:AS:662:U:H5'    | 6:AY:108:ARG:HA   | 1.99                     | 0.44              |
| 1:AS:1410:G:C6    | 1:AS:1411:U:C4    | 3.05                     | 0.44              |
| 1:AS:1568:U:C4    | 1:AS:1569:C:H1'   | 2.52                     | 0.44              |
| 1:AS:2211:A:H2'   | 1:AS:2212:G:O4'   | 2.18                     | 0.44              |
| 1:AS:2394:U:H2'   | 1:AS:2395:U:C6    | 2.52                     | 0.44              |
| 1:AS:2557:G:N3    | 1:AS:2557:G:H2'   | 2.32                     | 0.44              |
| 80:BE:150:GLU:O   | 80:BE:154:ARG:HG3 | 2.17                     | 0.44              |
| 15:BH:20:LEU:HD22 | 15:BH:23:ASN:HA   | 2.00                     | 0.44              |
| 23:BP:11:SER:OG   | 23:BP:12:VAL:N    | 2.50                     | 0.44              |
| 46:CM:112:A:O2'   | 46:CM:113:U:H5'   | 2.16                     | 0.44              |
| 46:CM:1238:U:H2'  | 46:CM:1239:U:H6   | 1.82                     | 0.44              |
| 46:CM:1417:C:O2'  | 46:CM:1423:U:O4   | 2.20                     | 0.44              |
| 46:CM:1548:U:H2'  | 46:CM:1549:G:H8   | 1.82                     | 0.44              |
| 46:CM:1553:U:H5'' | 65:DF:39:GLY:H    | 1.82                     | 0.44              |
| 48:CO:64:ARG:H    | 48:CO:88:VAL:CG1  | 2.31                     | 0.44              |
| 48:CO:175:GLU:O   | 48:CO:187:LYS:HD3 | 2.17                     | 0.44              |
| 51:CR:51:ARG:HD3  | 51:CR:51:ARG:HA   | 1.77                     | 0.44              |
| 54:CU:28:ALA:HA   | 54:CU:31:LYS:HB2  | 1.99                     | 0.44              |
| 55:CV:39:GLY:O    | 55:CV:61:GLU:HG3  | 2.17                     | 0.44              |
| 79:DT:67:HIS:O    | 79:DT:68:ILE:C    | 2.57                     | 0.44              |
| 79:DT:162:GLN:H   | 79:DT:162:GLN:NE2 | 2.14                     | 0.44              |
| 79:DT:246:ARG:HD3 | 79:DT:248:TRP:CH2 | 2.52                     | 0.44              |
| 1:1:1851:U:H2'    | 1:1:1852:C:H6     | 1.82                     | 0.44              |
| 1:1:2442:U:O4     | 1:1:2472:A:H1'    | 2.17                     | 0.44              |
| 1:1:2485:U:C2     | 1:1:2486:U:C5     | 3.06                     | 0.44              |
| 1:1:2603:U:H2'    | 1:1:2604:G:H8     | 1.83                     | 0.44              |
| 1:1:2895:U:H2'    | 1:1:2896:U:C6     | 2.52                     | 0.44              |
| 7:m:125:VAL:HG11  | 7:m:199:ILE:HG21  | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:s:50:ALA:HB2    | 13:s:65:ILE:HG13   | 1.98                     | 0.44              |
| 16:v:91:GLN:O      | 16:v:93:LYS:NZ     | 2.50                     | 0.44              |
| 25:7:57:ARG:HH21   | 25:7:63:ILE:HG13   | 1.83                     | 0.44              |
| 46:B:989:U:H3'     | 46:B:990:A:C5'     | 2.47                     | 0.44              |
| 46:B:1202:A:N3     | 57:M:27:PHE:HD2    | 2.15                     | 0.44              |
| 56:L:101:PRO:O     | 56:L:105:LEU:HD12  | 2.18                     | 0.44              |
| 59:O:62:LEU:HD22   | 59:O:75:VAL:CG1    | 2.48                     | 0.44              |
| 59:O:105:GLN:HG3   | 59:O:113:ARG:HD3   | 1.99                     | 0.44              |
| 63:S:114:THR:HA    | 63:S:117:VAL:O     | 2.17                     | 0.44              |
| 67:W:25:LEU:HD23   | 67:W:113:VAL:HG22  | 1.99                     | 0.44              |
| 76:f:12:ARG:HB2    | 76:f:12:ARG:NH1    | 2.31                     | 0.44              |
| 79:AR:67:HIS:CG    | 79:AR:68:ILE:H     | 2.35                     | 0.44              |
| 1:AS:412:G:O2'     | 18:BK:118:GLN:HB2  | 2.17                     | 0.44              |
| 1:AS:663:A:OP1     | 16:BI:203:ARG:HD2  | 2.17                     | 0.44              |
| 1:AS:896:G:H1'     | 1:AS:1585:A:N6     | 2.33                     | 0.44              |
| 1:AS:922:A:H2'     | 1:AS:923:C:H6      | 1.83                     | 0.44              |
| 1:AS:954:C:H5''    | 1:AS:2772:G:P      | 2.57                     | 0.44              |
| 1:AS:2210:A:H2'    | 1:AS:2211:A:H8     | 1.81                     | 0.44              |
| 6:AY:140:GLY:O     | 6:AY:142:ARG:NH1   | 2.51                     | 0.44              |
| 14:BG:155:GLU:OE1  | 29:BV:101:VAL:HG11 | 2.16                     | 0.44              |
| 42:CI:8:LYS:HE3    | 42:CI:12:ARG:NH2   | 2.33                     | 0.44              |
| 45:CL:96:LYS:HA    | 46:CM:575:G:O6     | 2.17                     | 0.44              |
| 46:CM:164:C:O2'    | 53:CT:133:LEU:O    | 2.31                     | 0.44              |
| 46:CM:390:G:H5''   | 46:CM:1716:C:O2'   | 2.17                     | 0.44              |
| 46:CM:1314:A:OP2   | 50:CQ:161:SER:OG   | 2.22                     | 0.44              |
| 46:CM:1523:G:OP1   | 72:DM:36:ALA:HB2   | 2.17                     | 0.44              |
| 47:CN:48:ILE:CG2   | 47:CN:161:PRO:HB2  | 2.47                     | 0.44              |
| 49:CP:30:TRP:CZ2   | 49:CP:32:PRO:HB3   | 2.52                     | 0.44              |
| 52:CS:65:ARG:O     | 52:CS:67:PRO:HD3   | 2.17                     | 0.44              |
| 53:CT:211:LEU:HD23 | 53:CT:215:ARG:HG2  | 2.00                     | 0.44              |
| 55:CV:62:THR:OG1   | 55:CV:75:LYS:HE3   | 2.18                     | 0.44              |
| 58:CY:16:GLN:OE1   | 58:CY:34:TRP:HB3   | 2.17                     | 0.44              |
| 60:DA:93:LYS:HB2   | 60:DA:150:VAL:HG11 | 1.98                     | 0.44              |
| 62:DC:127:ARG:O    | 62:DC:129:GLY:N    | 2.50                     | 0.44              |
| 69:DJ:28:ARG:HD2   | 69:DJ:60:LYS:HE2   | 1.99                     | 0.44              |
| 79:DT:113:SER:HB2  | 79:DT:154:ALA:HA   | 1.99                     | 0.44              |
| 79:DT:179:ASP:HB2  | 79:DT:186:ASN:ND2  | 2.29                     | 0.44              |
| 79:DT:231:LEU:HD12 | 79:DT:232:GLU:H    | 1.82                     | 0.44              |
| 79:DT:270:GLU:C    | 79:DT:272:LYS:H    | 2.24                     | 0.44              |
| 1:1:1755:U:C2'     | 1:1:1756:A:H5'     | 2.48                     | 0.44              |
| 1:1:3334:G:C6      | 25:7:56:ARG:HD2    | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:l:27:PHE:HE1     | 6:l:259:LEU:HD13   | 1.82                     | 0.44              |
| 10:p:74:PRO:HD3    | 10:p:234:TRP:CE2   | 2.52                     | 0.44              |
| 10:p:210:ALA:HA    | 10:p:213:SER:OG    | 2.17                     | 0.44              |
| 27:9:87:LYS:HB2    | 27:9:97:ILE:HD11   | 2.00                     | 0.44              |
| 28:AA:17:ARG:HD3   | 35:AH:73:GLN:HB3   | 1.99                     | 0.44              |
| 36:AI:22:VAL:O     | 36:AI:26:GLN:HG3   | 2.18                     | 0.44              |
| 45:i:98:ASP:O      | 45:i:99:SER:HB3    | 2.17                     | 0.44              |
| 46:B:1669:U:O4     | 46:B:1707:G:N2     | 2.51                     | 0.44              |
| 46:B:1749:A:H1'    | 46:B:1770:C:H5'    | 1.98                     | 0.44              |
| 73:c:3:LYS:NZ      | 73:c:6:ALA:HA      | 2.32                     | 0.44              |
| 79:AR:152:VAL:HG12 | 79:AR:170:SER:HB2  | 2.00                     | 0.44              |
| 79:AR:202:SER:HB3  | 79:AR:207:LEU:HB2  | 1.99                     | 0.44              |
| 1:AS:412:G:H2'     | 1:AS:413:U:C6      | 2.53                     | 0.44              |
| 1:AS:520:G:C6      | 1:AS:521:G:C5      | 3.05                     | 0.44              |
| 1:AS:649:G:C6      | 1:AS:650:G:C6      | 3.06                     | 0.44              |
| 1:AS:689:A:N1      | 3:AU:28:C:O2'      | 2.42                     | 0.44              |
| 1:AS:851:U:H2'     | 1:AS:852:G:C8      | 2.51                     | 0.44              |
| 1:AS:897:G:OP1     | 38:CE:12:HIS:NE2   | 2.48                     | 0.44              |
| 1:AS:972:U:H2'     | 1:AS:973:C:O4'     | 2.17                     | 0.44              |
| 1:AS:1153:G:H5''   | 9:BB:217:PHE:CE2   | 2.52                     | 0.44              |
| 1:AS:1317:G:H2'    | 1:AS:1318:U:O4'    | 2.17                     | 0.44              |
| 1:AS:1552:C:H5''   | 1:AS:2147:G:N2     | 2.31                     | 0.44              |
| 1:AS:1777:C:H2'    | 1:AS:1778:U:C6     | 2.52                     | 0.44              |
| 1:AS:2126:U:H2'    | 1:AS:2127:A:C8     | 2.53                     | 0.44              |
| 1:AS:2182:C:H2'    | 1:AS:2183:U:C6     | 2.52                     | 0.44              |
| 1:AS:2374:G:OP1    | 1:AS:2375:A:O2'    | 2.17                     | 0.44              |
| 1:AS:2603:U:H2'    | 1:AS:2604:G:C8     | 2.52                     | 0.44              |
| 1:AS:2680:C:H2'    | 1:AS:2681:C:C6     | 2.53                     | 0.44              |
| 1:AS:3061:C:H2'    | 1:AS:3062:U:O4'    | 2.18                     | 0.44              |
| 6:AY:54:ALA:HB3    | 6:AY:57:ALA:HB2    | 1.99                     | 0.44              |
| 10:BC:57:VAL:O     | 10:BC:61:ARG:HG3   | 2.18                     | 0.44              |
| 11:BD:17:THR:OG1   | 11:BD:28:THR:HB    | 2.16                     | 0.44              |
| 11:BD:47:LYS:NZ    | 11:BD:50:ASN:HA    | 2.33                     | 0.44              |
| 27:BT:27:ARG:NH1   | 27:BT:76:LEU:HA    | 2.32                     | 0.44              |
| 39:CF:73:LEU:HD12  | 39:CF:73:LEU:H     | 1.83                     | 0.44              |
| 45:CL:75:PRO:HG2   | 62:DC:130:ARG:O    | 2.17                     | 0.44              |
| 45:CL:96:LYS:HA    | 46:CM:575:G:C6     | 2.53                     | 0.44              |
| 46:CM:578:A:H5''   | 50:CQ:144:ARG:HH21 | 1.82                     | 0.44              |
| 46:CM:756:A:H4'    | 56:CW:7:THR:O      | 2.18                     | 0.44              |
| 46:CM:1167:U:H4'   | 62:DC:124:THR:HB   | 2.00                     | 0.44              |
| 46:CM:1535:G:O3'   | 65:DF:90:LYS:HD3   | 2.16                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:CS:55:ASP:O     | 52:CS:59:VAL:HG23  | 2.18                     | 0.44              |
| 52:CS:58:LEU:HD22  | 52:CS:168:VAL:HG23 | 1.99                     | 0.44              |
| 54:CU:21:PHE:N     | 54:CU:21:PHE:CD1   | 2.85                     | 0.44              |
| 57:CX:5:LYS:HZ2    | 59:CZ:43:ARG:HH22  | 1.66                     | 0.44              |
| 57:CX:18:GLU:H     | 57:CX:89:LEU:HB3   | 1.83                     | 0.44              |
| 59:CZ:135:ILE:HA   | 59:CZ:138:GLU:OE2  | 2.17                     | 0.44              |
| 60:DA:4:MET:HE1    | 60:DA:121:ARG:HG3  | 2.00                     | 0.44              |
| 68:DI:5:LYS:HB3    | 68:DI:7:GLN:OE1    | 2.17                     | 0.44              |
| 79:DT:19:TRP:HB3   | 79:DT:287:ILE:HD11 | 1.99                     | 0.44              |
| 79:DT:133:LYS:HD3  | 79:DT:141:CYS:SG   | 2.57                     | 0.44              |
| 79:DT:155:VAL:HG12 | 79:DT:168:SER:CB   | 2.47                     | 0.44              |
| 79:DT:234:LYS:HD2  | 79:DT:255:SER:CB   | 2.48                     | 0.44              |
| 82:12:103:ASN:CB   | 82:12:105:PRO:HD3  | 2.48                     | 0.44              |
| 1:1:149:A:C4       | 1:1:150:A:C8       | 3.05                     | 0.44              |
| 1:1:163:A:H2'      | 1:1:164:U:O4'      | 2.17                     | 0.44              |
| 1:1:976:A:N6       | 1:1:1100:G:O2'     | 2.36                     | 0.44              |
| 1:1:983:U:H2'      | 1:1:984:U:C6       | 2.52                     | 0.44              |
| 1:1:1291:G:H2'     | 1:1:1292:C:C6      | 2.52                     | 0.44              |
| 1:1:1801:C:H2'     | 1:1:1802:A:H8      | 1.81                     | 0.44              |
| 1:1:2902:A:H2'     | 1:1:2903:C:C6      | 2.53                     | 0.44              |
| 1:1:3185:G:C6      | 1:1:3231:G:C6      | 3.06                     | 0.44              |
| 1:1:3322:U:H2'     | 1:1:3323:U:C6      | 2.53                     | 0.44              |
| 1:1:3336:G:H2'     | 1:1:3337:A:H8      | 1.83                     | 0.44              |
| 5:k:107:ALA:HB1    | 5:k:200:GLU:HG3    | 2.00                     | 0.44              |
| 9:o:212:PHE:HB3    | 9:o:225:ASP:OD2    | 2.18                     | 0.44              |
| 36:AI:63:ARG:O     | 36:AI:67:ARG:HG3   | 2.16                     | 0.44              |
| 40:AM:41:ARG:HD2   | 40:AM:41:ARG:HA    | 1.79                     | 0.44              |
| 45:i:113:ARG:HE    | 45:i:113:ARG:HB2   | 1.55                     | 0.44              |
| 46:B:91:G:H2'      | 46:B:92:A:O4'      | 2.17                     | 0.44              |
| 46:B:112:A:O2'     | 46:B:113:U:H5'     | 2.17                     | 0.44              |
| 46:B:327:G:H2'     | 46:B:328:G:H8      | 1.83                     | 0.44              |
| 46:B:1293:G:H2'    | 46:B:1294:C:C6     | 2.53                     | 0.44              |
| 46:B:1571:G:N7     | 63:S:13:LYS:HE2    | 2.33                     | 0.44              |
| 51:G:162:ILE:HG22  | 51:G:164:LEU:H     | 1.83                     | 0.44              |
| 54:J:37:LEU:HD22   | 54:J:66:TYR:CE1    | 2.52                     | 0.44              |
| 62:R:25:LEU:HG     | 62:R:87:PRO:HB3    | 1.99                     | 0.44              |
| 75:e:42:ARG:NH1    | 75:e:58:GLU:O      | 2.50                     | 0.44              |
| 79:AR:133:LYS:HD3  | 79:AR:141:CYS:SG   | 2.57                     | 0.44              |
| 79:AR:195:TYR:O    | 79:AR:212:GLY:HA3  | 2.18                     | 0.44              |
| 1:AS:114:A:H5''    | 16:BI:4:TYR:HB2    | 2.00                     | 0.44              |
| 1:AS:239:A:OP1     | 36:CC:94:LYS:NZ    | 2.35                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:269:G:P       | 16:BI:44:ARG:HH12  | 2.40                     | 0.44              |
| 1:AS:528:A:O2'     | 1:AS:529:A:H5'     | 2.18                     | 0.44              |
| 1:AS:813:A:OP1     | 38:CE:30:GLN:NE2   | 2.23                     | 0.44              |
| 1:AS:849:G:N7      | 44:CK:2:THR:HG23   | 2.33                     | 0.44              |
| 1:AS:1027:C:H2'    | 1:AS:1028:C:C6     | 2.53                     | 0.44              |
| 1:AS:1761:U:H2'    | 1:AS:1762:G:C4'    | 2.48                     | 0.44              |
| 1:AS:1787:U:H2'    | 1:AS:1788:C:C6     | 2.52                     | 0.44              |
| 1:AS:2581:A:H2'    | 1:AS:2582:G:C8     | 2.53                     | 0.44              |
| 1:AS:3164:U:H1'    | 1:AS:3165:U:C5     | 2.53                     | 0.44              |
| 1:AS:3176:C:H2'    | 1:AS:3177:C:C6     | 2.52                     | 0.44              |
| 4:AW:54:ARG:HG2    | 4:AW:56:ALA:H      | 1.83                     | 0.44              |
| 6:AY:136:VAL:HA    | 6:AY:246:GLY:O     | 2.18                     | 0.44              |
| 6:AY:139:ARG:NH2   | 6:AY:241:PRO:HB2   | 2.33                     | 0.44              |
| 6:AY:204:ARG:CZ    | 6:AY:241:PRO:HB3   | 2.48                     | 0.44              |
| 7:AZ:51:LEU:HB2    | 7:AZ:144:VAL:CG1   | 2.47                     | 0.44              |
| 10:BC:194:LYS:HG3  | 10:BC:195:THR:HG23 | 1.99                     | 0.44              |
| 11:BD:86:TYR:CE2   | 11:BD:151:LEU:HB2  | 2.53                     | 0.44              |
| 13:BF:25:GLU:OE2   | 13:BF:29:ARG:HD3   | 2.18                     | 0.44              |
| 13:BF:47:GLN:OE1   | 13:BF:64:LYS:HD3   | 2.17                     | 0.44              |
| 14:BG:52:ASP:OD1   | 14:BG:143:VAL:N    | 2.51                     | 0.44              |
| 15:BH:14:GLU:HG2   | 15:BH:17:ARG:CG    | 2.45                     | 0.44              |
| 16:BI:144:ARG:HG2  | 36:CC:95:PHE:HE2   | 1.83                     | 0.44              |
| 22:BO:130:ARG:HG2  | 22:BO:130:ARG:HH11 | 1.83                     | 0.44              |
| 25:BR:99:SER:HA    | 25:BR:102:LYS:HD3  | 1.99                     | 0.44              |
| 27:BT:85:LEU:HD23  | 27:BT:85:LEU:HA    | 1.76                     | 0.44              |
| 46:CM:485:G:C4     | 46:CM:486:G:C8     | 3.05                     | 0.44              |
| 46:CM:938:G:H2'    | 46:CM:939:G:C8     | 2.53                     | 0.44              |
| 46:CM:952:A:OP2    | 60:DA:124:ARG:NH2  | 2.51                     | 0.44              |
| 46:CM:1308:C:H2'   | 46:CM:1309:G:O4'   | 2.17                     | 0.44              |
| 46:CM:1369:G:C8    | 46:CM:1370:A:C8    | 3.06                     | 0.44              |
| 49:CP:36:LEU:HD21  | 49:CP:51:ILE:HD12  | 2.00                     | 0.44              |
| 50:CQ:139:ILE:HG12 | 50:CQ:185:ILE:HG22 | 1.98                     | 0.44              |
| 52:CS:73:THR:N     | 52:CS:91:GLU:OE2   | 2.39                     | 0.44              |
| 52:CS:143:ARG:HB2  | 52:CS:218:GLU:OE2  | 2.18                     | 0.44              |
| 52:CS:196:GLU:O    | 52:CS:200:ASN:OD1  | 2.34                     | 0.44              |
| 53:CT:102:VAL:HG13 | 53:CT:106:LEU:HD12 | 1.98                     | 0.44              |
| 55:CV:101:VAL:HG22 | 55:CV:174:VAL:HG22 | 2.00                     | 0.44              |
| 59:CZ:29:LYS:N     | 59:CZ:100:TRP:CZ3  | 2.86                     | 0.44              |
| 75:DP:38:ARG:O     | 75:DP:40:ILE:HG12  | 2.17                     | 0.44              |
| 78:DS:123:LYS:HD3  | 78:DS:125:LYS:HE3  | 1.98                     | 0.44              |
| 79:DT:19:TRP:CE2   | 79:DT:303:THR:HB   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:DT:80:TYR:HD2  | 79:DT:92:LEU:HD11 | 1.82                     | 0.44              |
| 81:P0:55:LYS:HG2  | 84:P0:401:MG:MG   | 1.43                     | 0.44              |
| 82:12:103:ASN:CA  | 82:12:144:ASP:HA  | 2.38                     | 0.44              |
| 1:1:21:G:H1'      | 3:4:104:A:N3      | 2.32                     | 0.44              |
| 1:1:150:A:C5      | 1:1:151:U:C5      | 3.05                     | 0.44              |
| 1:1:691:A:O2'     | 6:1:235:GLY:HA3   | 2.17                     | 0.44              |
| 1:1:1696:G:H2'    | 1:1:1697:C:C6     | 2.53                     | 0.44              |
| 15:u:19:VAL:HG11  | 15:u:55:ILE:HD12  | 1.99                     | 0.44              |
| 27:9:39:LEU:HD12  | 27:9:106:ILE:O    | 2.18                     | 0.44              |
| 27:9:45:VAL:CG1   | 27:9:46:LYS:H     | 2.24                     | 0.44              |
| 40:AM:9:THR:O     | 40:AM:13:LEU:HG   | 2.18                     | 0.44              |
| 46:B:36:C:H2'     | 46:B:37:U:C6      | 2.53                     | 0.44              |
| 46:B:479:A:H2'    | 46:B:480:U:H6     | 1.82                     | 0.44              |
| 46:B:685:C:H5''   | 69:Y:119:LYS:HG2  | 1.99                     | 0.44              |
| 46:B:813:U:H5'    | 46:B:813:U:H6     | 1.83                     | 0.44              |
| 46:B:822:G:H3'    | 46:B:823:G:C4'    | 2.48                     | 0.44              |
| 46:B:1133:C:H2'   | 46:B:1134:G:C8    | 2.53                     | 0.44              |
| 46:B:1289:G:H5'   | 46:B:1307:A:OP2   | 2.18                     | 0.44              |
| 52:H:26:ALA:HB3   | 63:S:26:GLY:O     | 2.17                     | 0.44              |
| 56:L:109:LEU:O    | 56:L:113:VAL:HG23 | 2.17                     | 0.44              |
| 61:Q:98:ARG:HD2   | 73:c:49:ALA:HB2   | 1.98                     | 0.44              |
| 63:S:21:VAL:HG22  | 63:S:64:ILE:HG12  | 1.99                     | 0.44              |
| 74:d:12:PRO:HA    | 74:d:15:GLU:HB3   | 1.99                     | 0.44              |
| 1:AS:538:G:C2     | 1:AS:539:G:C6     | 3.06                     | 0.44              |
| 1:AS:1029:U:H2'   | 1:AS:1030:U:C6    | 2.53                     | 0.44              |
| 1:AS:1467:U:OP1   | 20:BM:5:ARG:NH2   | 2.51                     | 0.44              |
| 1:AS:2184:G:H4'   | 1:AS:2185:A:C5    | 2.53                     | 0.44              |
| 1:AS:2269:A:N3    | 46:CM:1642:A:H2   | 2.16                     | 0.44              |
| 1:AS:2367:C:O2'   | 1:AS:3272:A:N1    | 2.49                     | 0.44              |
| 1:AS:2530:C:N4    | 31:BX:59:GLU:OE2  | 2.50                     | 0.44              |
| 1:AS:3339:U:H2'   | 1:AS:3343:C:N4    | 2.32                     | 0.44              |
| 6:AY:42:ARG:O     | 6:AY:46:ASN:ND2   | 2.49                     | 0.44              |
| 6:AY:59:HIS:CE1   | 6:AY:99:ARG:HD2   | 2.52                     | 0.44              |
| 20:BM:134:HIS:HE1 | 20:BM:136:ARG:NE  | 2.12                     | 0.44              |
| 32:BY:71:ARG:NH1  | 32:BY:103:LEU:HB3 | 2.33                     | 0.44              |
| 36:CC:118:ILE:O   | 36:CC:119:LYS:C   | 2.60                     | 0.44              |
| 46:CM:75:U:H2'    | 46:CM:76:A:C4     | 2.53                     | 0.44              |
| 46:CM:246:U:H4'   | 58:CY:36:LYS:HD3  | 1.99                     | 0.44              |
| 46:CM:283:G:H2'   | 46:CM:284:C:C6    | 2.53                     | 0.44              |
| 46:CM:1204:A:N3   | 57:CX:51:SER:OG   | 2.43                     | 0.44              |
| 46:CM:1237:C:H2'  | 46:CM:1238:U:O4'  | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:1300:U:O2'   | 46:CM:1301:G:H8    | 2.01                     | 0.44              |
| 52:CS:163:SER:OG   | 75:DP:46:GLY:HA3   | 2.18                     | 0.44              |
| 57:CX:4:PRO:HG2    | 57:CX:7:ASP:HB2    | 1.99                     | 0.44              |
| 59:CZ:102:GLY:O    | 59:CZ:104:CYS:N    | 2.44                     | 0.44              |
| 65:DF:46:VAL:HG12  | 65:DF:72:ILE:HG22  | 1.99                     | 0.44              |
| 65:DF:109:LEU:O    | 65:DF:113:LEU:HG   | 2.17                     | 0.44              |
| 79:DT:20:VAL:O     | 79:DT:288:SER:HB2  | 2.18                     | 0.44              |
| 79:DT:262:LEU:HD23 | 79:DT:265:ARG:HH11 | 1.81                     | 0.44              |
| 81:P0:16:ARG:HD3   | 81:P0:66:PHE:CD2   | 2.53                     | 0.44              |
| 1:1:528:A:O2'      | 1:1:529:A:H5'      | 2.18                     | 0.44              |
| 1:1:624:U:H2'      | 1:1:625:C:C6       | 2.52                     | 0.44              |
| 1:1:689:A:N6       | 6:l:49:GLN:OE1     | 2.51                     | 0.44              |
| 1:1:1478:A:H4'     | 1:1:1479:G:OP2     | 2.18                     | 0.44              |
| 1:1:1791:U:OP1     | 4:j:191:VAL:HG11   | 2.18                     | 0.44              |
| 1:1:2108:G:H1'     | 1:1:2122:A:H5''    | 2.00                     | 0.44              |
| 1:1:2115:U:C6      | 1:1:2119:U:C4      | 3.06                     | 0.44              |
| 1:1:2257:A:C8      | 1:1:2266:G:C8      | 3.06                     | 0.44              |
| 1:1:2796:G:C4      | 1:1:2797:C:C5      | 3.06                     | 0.44              |
| 3:4:23:U:OP1       | 27:9:16:ARG:NH1    | 2.51                     | 0.44              |
| 11:q:171:ASP:OD1   | 11:q:173:ARG:HB2   | 2.18                     | 0.44              |
| 14:t:191:GLU:O     | 14:t:194:GLU:HG3   | 2.17                     | 0.44              |
| 24:6:37:LEU:HG     | 24:6:59:MET:O      | 2.18                     | 0.44              |
| 26:8:46:TYR:CD1    | 36:AI:75:TYR:HB3   | 2.52                     | 0.44              |
| 46:B:30:G:H2'      | 46:B:31:C:H6       | 1.81                     | 0.44              |
| 46:B:68:A:N6       | 53:I:132:ARG:HG2   | 2.32                     | 0.44              |
| 46:B:330:U:H5''    | 55:K:31:ARG:NH1    | 2.32                     | 0.44              |
| 46:B:399:A:O2'     | 46:B:400:C:H4'     | 2.16                     | 0.44              |
| 46:B:600:U:H2'     | 46:B:601:U:C6      | 2.53                     | 0.44              |
| 48:D:145:ARG:NH2   | 48:D:151:LYS:O     | 2.50                     | 0.44              |
| 50:F:63:GLN:OE1    | 50:F:65:ARG:NH2    | 2.49                     | 0.44              |
| 57:M:83:PRO:C      | 57:M:85:GLY:H      | 2.25                     | 0.44              |
| 59:O:130:SER:C     | 59:O:132:GLU:H     | 2.25                     | 0.44              |
| 66:V:27:LYS:HE3    | 66:V:111:ILE:HG23  | 1.99                     | 0.44              |
| 67:W:33:LEU:HG     | 67:W:88:ARG:HE     | 1.81                     | 0.44              |
| 78:h:157:GLU:HG3   | 78:h:159:LEU:HG    | 1.99                     | 0.44              |
| 1:AS:14:C:H5''     | 26:BS:42:ARG:HG2   | 1.98                     | 0.44              |
| 1:AS:169:G:C6      | 1:AS:249:G:H1'     | 2.53                     | 0.44              |
| 1:AS:407:A:C2      | 3:AU:17:A:H1'      | 2.53                     | 0.44              |
| 1:AS:975:U:H4'     | 1:AS:976:A:O4'     | 2.17                     | 0.44              |
| 1:AS:1291:G:H2'    | 1:AS:1292:C:C6     | 2.52                     | 0.44              |
| 1:AS:1443:G:OP1    | 18:BK:65:SER:HB2   | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:1762:G:H2'    | 1:AS:1763:C:H6     | 1.82                     | 0.44              |
| 1:AS:2170:C:O2'    | 1:AS:2290:A:N1     | 2.49                     | 0.44              |
| 1:AS:2201:A:H8     | 1:AS:2201:A:OP2    | 2.00                     | 0.44              |
| 1:AS:2485:U:H2'    | 1:AS:2486:U:H6     | 1.81                     | 0.44              |
| 1:AS:2956:C:H2'    | 1:AS:2957:C:C6     | 2.53                     | 0.44              |
| 1:AS:3005:A:H2'    | 1:AS:3006:C:C6     | 2.53                     | 0.44              |
| 1:AS:3146:G:OP1    | 34:CA:6:ARG:HB2    | 2.18                     | 0.44              |
| 2:AT:23:A:H1'      | 2:AT:121:U:H2'     | 1.98                     | 0.44              |
| 3:AU:65:A:P        | 36:CC:53:ARG:HE    | 2.40                     | 0.44              |
| 10:BC:153:LEU:HD22 | 10:BC:179:ALA:HB3  | 2.00                     | 0.44              |
| 17:BJ:13:LYS:HG3   | 17:BJ:41:GLU:HB3   | 2.00                     | 0.44              |
| 22:BO:39:ILE:HG12  | 22:BO:63:ILE:CD1   | 2.48                     | 0.44              |
| 22:BO:124:GLU:HG3  | 22:BO:125:THR:O    | 2.17                     | 0.44              |
| 46:CM:119:A:H1'    | 46:CM:395:A:C5     | 2.53                     | 0.44              |
| 46:CM:721:C:N4     | 46:CM:722:A:H62    | 2.15                     | 0.44              |
| 46:CM:873:U:H2'    | 46:CM:874:U:C6     | 2.52                     | 0.44              |
| 46:CM:1131:G:H2'   | 46:CM:1132:A:H8    | 1.82                     | 0.44              |
| 46:CM:1262:G:O3'   | 50:CQ:184:GLY:HA3  | 2.17                     | 0.44              |
| 46:CM:1556:A:H2'   | 46:CM:1557:A:C8    | 2.53                     | 0.44              |
| 46:CM:1784:A:C2    | 73:DN:98:PRO:HG3   | 2.53                     | 0.44              |
| 48:CO:119:SER:HB2  | 48:CO:143:THR:HG21 | 1.99                     | 0.44              |
| 48:CO:133:TYR:CD2  | 48:CO:181:LEU:HD13 | 2.53                     | 0.44              |
| 52:CS:32:ASP:OD1   | 52:CS:33:VAL:N     | 2.51                     | 0.44              |
| 54:CU:25:GLU:O     | 54:CU:31:LYS:CD    | 2.65                     | 0.44              |
| 64:DE:103:ASP:OD2  | 64:DE:105:ASP:HB2  | 2.18                     | 0.44              |
| 70:DK:29:TYR:HA    | 70:DK:32:ARG:NH1   | 2.33                     | 0.44              |
| 72:DM:100:ILE:C    | 72:DM:101:TYR:HD1  | 2.25                     | 0.44              |
| 81:P0:57:THR:HA    | 81:P0:60:ARG:HD2   | 1.99                     | 0.44              |
| 1:1:350:C:N3       | 1:1:368:G:H5'      | 2.33                     | 0.44              |
| 1:1:594:C:H2'      | 1:1:595:G:O4'      | 2.18                     | 0.44              |
| 1:1:2589:U:OP1     | 30:AC:3:LYS:HA     | 2.18                     | 0.44              |
| 1:1:2957:C:H2'     | 1:1:2958:U:C6      | 2.53                     | 0.44              |
| 1:1:3151:C:H2'     | 1:1:3152:G:C8      | 2.53                     | 0.44              |
| 8:n:22:LYS:HA      | 8:n:22:LYS:HD3     | 1.78                     | 0.44              |
| 46:B:141:G:H2'     | 46:B:142:G:C8      | 2.53                     | 0.44              |
| 46:B:180:A:H2'     | 46:B:181:U:C6      | 2.53                     | 0.44              |
| 46:B:341:C:H2'     | 46:B:342:A:H8      | 1.83                     | 0.44              |
| 46:B:861:G:H2'     | 46:B:921:G:N2      | 2.33                     | 0.44              |
| 46:B:987:G:N2      | 46:B:1747:G:O3'    | 2.51                     | 0.44              |
| 46:B:1720:C:H2'    | 46:B:1721:U:C6     | 2.51                     | 0.44              |
| 79:AR:246:ARG:NH1  | 79:AR:296:GLN:OE1  | 2.36                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AS:615:G:H2'    | 1:AS:616:C:C6      | 2.53                     | 0.44              |
| 1:AS:814:C:H2'    | 1:AS:815:U:O4'     | 2.18                     | 0.44              |
| 1:AS:1941:A:H2'   | 1:AS:1942:A:H8     | 1.83                     | 0.44              |
| 1:AS:2668:A:H2'   | 1:AS:2669:A:C8     | 2.53                     | 0.44              |
| 15:BH:62:LEU:HD22 | 15:BH:65:LEU:HB2   | 2.00                     | 0.44              |
| 17:BJ:4:PHE:CE2   | 34:CA:33:GLU:HB2   | 2.52                     | 0.44              |
| 26:BS:25:LYS:O    | 26:BS:27:ARG:HG3   | 2.17                     | 0.44              |
| 26:BS:70:GLU:O    | 26:BS:74:LYS:HG3   | 2.18                     | 0.44              |
| 34:CA:106:ASN:ND2 | 34:CA:106:ASN:O    | 2.51                     | 0.44              |
| 46:CM:254:A:H2'   | 46:CM:255:A:O4'    | 2.18                     | 0.44              |
| 46:CM:517:C:H6    | 46:CM:517:C:H2'    | 1.61                     | 0.44              |
| 46:CM:908:A:H2'   | 46:CM:909:A:H8     | 1.83                     | 0.44              |
| 46:CM:1354:U:C2   | 46:CM:1355:A:N7    | 2.86                     | 0.44              |
| 46:CM:1457:A:C2   | 46:CM:1460:G:N3    | 2.83                     | 0.44              |
| 46:CM:1485:G:O6   | 46:CM:1496:C:N4    | 2.36                     | 0.44              |
| 46:CM:1521:G:N2   | 52:CS:187:ILE:HG13 | 2.33                     | 0.44              |
| 46:CM:1588:G:N2   | 66:DG:88:PHE:HB3   | 2.33                     | 0.44              |
| 46:CM:1763:A:H2'  | 46:CM:1764:G:C8    | 2.53                     | 0.44              |
| 47:CN:23:HIS:O    | 47:CN:48:ILE:HD12  | 2.17                     | 0.44              |
| 48:CO:88:VAL:HG21 | 48:CO:96:LEU:HD23  | 2.00                     | 0.44              |
| 53:CT:28:TYR:CZ   | 53:CT:104:GLN:HG3  | 2.52                     | 0.44              |
| 54:CU:14:GLU:HG2  | 54:CU:42:ILE:HB    | 2.00                     | 0.44              |
| 57:CX:15:LEU:O    | 57:CX:19:GLY:HA2   | 2.18                     | 0.44              |
| 62:DC:32:GLU:HA   | 62:DC:35:LYS:HD3   | 2.00                     | 0.44              |
| 65:DF:82:PRO:HG2  | 66:DG:36:ILE:HG21  | 2.00                     | 0.44              |
| 68:DI:37:ALA:HA   | 68:DI:50:ASN:OD1   | 2.18                     | 0.44              |
| 79:DT:44:LYS:O    | 79:DT:59:LYS:HB2   | 2.17                     | 0.44              |
| 79:DT:169:ALA:CB  | 79:DT:199:ILE:HD11 | 2.40                     | 0.44              |
| 79:DT:206:SER:CB  | 79:DT:223:ASN:HD22 | 2.18                     | 0.44              |
| 81:P0:107:ALA:HB1 | 81:P0:108:PRO:CD   | 2.48                     | 0.44              |
| 1:1:1892:A:N6     | 1:1:2317:C:H42     | 2.11                     | 0.43              |
| 1:1:2330:A:H2'    | 1:1:2331:G:H8      | 1.83                     | 0.43              |
| 1:1:2492:U:O2     | 1:1:2565:A:N6      | 2.49                     | 0.43              |
| 1:1:3257:A:C5     | 1:1:3258:U:C4      | 3.06                     | 0.43              |
| 2:3:108:U:H2'     | 2:3:109:U:C6       | 2.53                     | 0.43              |
| 17:w:83:LYS:HB3   | 17:w:83:LYS:HE2    | 1.77                     | 0.43              |
| 25:7:108:LYS:HG2  | 25:7:112:ASP:OD2   | 2.18                     | 0.43              |
| 32:AE:52:PRO:O    | 32:AE:56:ILE:HG12  | 2.18                     | 0.43              |
| 45:i:114:GLU:OE1  | 45:i:114:GLU:N     | 2.50                     | 0.43              |
| 46:B:397:A:H4'    | 51:G:3:ARG:HG2     | 1.99                     | 0.43              |
| 46:B:1105:U:H2'   | 46:B:1106:C:C6     | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:1219:A:OP2   | 46:B:1230:G:O2'   | 2.14                     | 0.43              |
| 46:B:1498:G:H2'   | 46:B:1499:G:C8    | 2.52                     | 0.43              |
| 46:B:1739:U:H2'   | 46:B:1740:A:C8    | 2.51                     | 0.43              |
| 46:B:1763:A:H2'   | 46:B:1764:G:H8    | 1.82                     | 0.43              |
| 49:E:45:ILE:HD11  | 49:E:234:PRO:HB2  | 1.98                     | 0.43              |
| 49:E:107:GLY:HA2  | 49:E:210:PHE:HE2  | 1.83                     | 0.43              |
| 50:F:36:ALA:HA    | 50:F:100:ALA:HB3  | 1.99                     | 0.43              |
| 67:W:22:ARG:NE    | 67:W:91:ASP:OD1   | 2.46                     | 0.43              |
| 1:AS:640:U:O2'    | 1:AS:642:G:N7     | 2.40                     | 0.43              |
| 1:AS:657:G:H2'    | 1:AS:1428:C:H42   | 1.82                     | 0.43              |
| 1:AS:1199:A:H2'   | 1:AS:1200:A:H8    | 1.78                     | 0.43              |
| 1:AS:1468:U:H5'   | 20:BM:4:LEU:HB2   | 1.99                     | 0.43              |
| 1:AS:1478:A:H4'   | 1:AS:1479:G:OP2   | 2.18                     | 0.43              |
| 1:AS:1922:C:H5''  | 44:CK:8:VAL:CG1   | 2.48                     | 0.43              |
| 1:AS:2345:A:H2'   | 1:AS:2346:A:H8    | 1.79                     | 0.43              |
| 1:AS:2397:A:H2'   | 1:AS:2398:C:H6    | 1.83                     | 0.43              |
| 1:AS:2430:G:O2'   | 1:AS:2431:U:OP2   | 2.31                     | 0.43              |
| 1:AS:2485:U:C2    | 1:AS:2486:U:C5    | 3.06                     | 0.43              |
| 3:AU:4:C:H2'      | 3:AU:5:U:H6       | 1.83                     | 0.43              |
| 3:AU:140:G:O3'    | 16:BI:109:ARG:NH1 | 2.51                     | 0.43              |
| 4:AW:145:LYS:HD3  | 4:AW:159:SER:HA   | 2.00                     | 0.43              |
| 5:AX:284:ARG:NH2  | 5:AX:295:ALA:O    | 2.51                     | 0.43              |
| 9:BB:134:TYR:CZ   | 9:BB:228:ASN:HB2  | 2.53                     | 0.43              |
| 11:BD:89:LYS:O    | 11:BD:182:SER:N   | 2.45                     | 0.43              |
| 11:BD:137:SER:HB3 | 11:BD:143:GLU:HB3 | 2.00                     | 0.43              |
| 14:BG:190:LYS:HE3 | 14:BG:190:LYS:HB2 | 1.69                     | 0.43              |
| 18:BK:14:SER:HA   | 18:BK:150:LEU:O   | 2.18                     | 0.43              |
| 25:BR:113:LYS:O   | 25:BR:116:LYS:HB2 | 2.18                     | 0.43              |
| 28:BU:38:PHE:CD1  | 28:BU:76:ASN:HB2  | 2.52                     | 0.43              |
| 28:BU:42:ILE:HD13 | 28:BU:98:SER:HA   | 2.00                     | 0.43              |
| 36:CC:84:LYS:HB3  | 38:CE:78:PHE:CG   | 2.52                     | 0.43              |
| 39:CF:33:ALA:C    | 39:CF:35:GLY:H    | 2.26                     | 0.43              |
| 46:CM:165:U:H2'   | 46:CM:166:A:H5''  | 2.00                     | 0.43              |
| 46:CM:290:U:H2'   | 46:CM:291:U:C6    | 2.52                     | 0.43              |
| 46:CM:348:U:OP1   | 46:CM:349:C:O2'   | 2.30                     | 0.43              |
| 46:CM:810:U:C4    | 46:CM:811:U:C4    | 3.06                     | 0.43              |
| 46:CM:881:U:O2    | 61:DB:36:ARG:NH1  | 2.51                     | 0.43              |
| 46:CM:1143:C:O2'  | 46:CM:1568:C:OP2  | 2.35                     | 0.43              |
| 46:CM:1664:C:H2'  | 46:CM:1665:C:C6   | 2.54                     | 0.43              |
| 53:CT:57:ASP:O    | 53:CT:107:SER:OG  | 2.24                     | 0.43              |
| 54:CU:46:ASP:HB2  | 54:CU:52:LYS:HG2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:DC:17:PHE:CE2  | 62:DC:36:LEU:HD12 | 2.53                     | 0.43              |
| 65:DF:6:GLN:OE1   | 65:DF:6:GLN:N     | 2.50                     | 0.43              |
| 70:DK:79:ASN:OD1  | 70:DK:79:ASN:N    | 2.51                     | 0.43              |
| 79:DT:84:ALA:HA   | 79:DT:90:LEU:HD23 | 1.99                     | 0.43              |
| 81:P0:15:LEU:HD12 | 81:P0:52:LEU:HD21 | 2.00                     | 0.43              |
| 1:1:816:A:H2'     | 1:1:817:U:C6      | 2.53                     | 0.43              |
| 1:1:976:A:H8      | 1:1:976:A:H3'     | 1.81                     | 0.43              |
| 1:1:1202:G:OP1    | 12:r:157:TYR:OH   | 2.27                     | 0.43              |
| 1:1:1218:G:OP1    | 81:P0:55:LYS:HD3  | 2.17                     | 0.43              |
| 1:1:1596:U:H5''   | 20:z:42:ARG:HH22  | 1.82                     | 0.43              |
| 1:1:1787:U:H2'    | 1:1:1788:C:C6     | 2.53                     | 0.43              |
| 1:1:2425:G:N1     | 1:1:2478:A:C2     | 2.86                     | 0.43              |
| 1:1:2785:A:H2'    | 1:1:2786:G:O4'    | 2.19                     | 0.43              |
| 1:1:2903:C:H2'    | 1:1:2904:U:O4'    | 2.18                     | 0.43              |
| 1:1:2915:G:H2'    | 1:1:2916:U:O4'    | 2.18                     | 0.43              |
| 1:1:3090:C:H2'    | 1:1:3091:U:O4'    | 2.17                     | 0.43              |
| 12:r:47:PRO:HB3   | 12:r:171:TRP:CZ2  | 2.52                     | 0.43              |
| 17:w:11:ASP:HB2   | 17:w:118:ARG:HB3  | 1.99                     | 0.43              |
| 46:B:368:A:H2'    | 46:B:369:G:C8     | 2.53                     | 0.43              |
| 46:B:1485:G:H4'   | 66:V:121:GLY:N    | 2.28                     | 0.43              |
| 46:B:1529:G:N2    | 46:B:1555:C:O2'   | 2.51                     | 0.43              |
| 50:F:19:TYR:CE1   | 50:F:38:VAL:HG13  | 2.53                     | 0.43              |
| 50:F:178:MET:HE3  | 50:F:183:LEU:HD12 | 1.99                     | 0.43              |
| 54:J:74:THR:HG22  | 54:J:88:PHE:HE1   | 1.83                     | 0.43              |
| 62:R:60:LEU:HD23  | 62:R:60:LEU:HA    | 1.84                     | 0.43              |
| 70:Z:89:ASN:HB2   | 70:Z:92:CYS:SG    | 2.59                     | 0.43              |
| 1:AS:522:C:C2     | 1:AS:523:G:C8     | 3.06                     | 0.43              |
| 1:AS:623:A:H2'    | 1:AS:624:U:H6     | 1.83                     | 0.43              |
| 1:AS:1186:A:H4'   | 41:CH:37:ARG:NH2  | 2.33                     | 0.43              |
| 1:AS:1909:A:N3    | 1:AS:2098:A:H2'   | 2.32                     | 0.43              |
| 1:AS:1936:G:OP1   | 20:BM:80:LYS:HE3  | 2.18                     | 0.43              |
| 1:AS:2108:G:H1'   | 1:AS:2122:A:H5''  | 1.99                     | 0.43              |
| 1:AS:3021:A:H1'   | 5:AX:54:THR:O     | 2.18                     | 0.43              |
| 1:AS:3023:U:C2    | 1:AS:3024:G:C8    | 3.05                     | 0.43              |
| 1:AS:3038:U:H2'   | 1:AS:3039:C:C6    | 2.54                     | 0.43              |
| 1:AS:3344:U:H4'   | 5:AX:315:GLY:HA2  | 1.99                     | 0.43              |
| 2:AT:96:U:O2      | 9:BB:222:GLN:NE2  | 2.49                     | 0.43              |
| 3:AU:4:C:C2       | 3:AU:5:U:C5       | 3.07                     | 0.43              |
| 7:AZ:4:GLN:HG3    | 7:AZ:5:LYS:N      | 2.33                     | 0.43              |
| 8:BA:39:LEU:HB3   | 8:BA:83:VAL:CG1   | 2.47                     | 0.43              |
| 8:BA:58:GLU:H     | 8:BA:58:GLU:CD    | 2.26                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BR:101:ARG:O    | 25:BR:102:LYS:C    | 2.61                     | 0.43              |
| 27:BT:52:GLN:O     | 27:BT:70:VAL:HB    | 2.19                     | 0.43              |
| 45:CL:82:LYS:NZ    | 46:CM:1163:G:H5''  | 2.33                     | 0.43              |
| 46:CM:156:U:O2'    | 46:CM:157:U:H3'    | 2.17                     | 0.43              |
| 46:CM:232:G:C5     | 46:CM:233:G:H1'    | 2.53                     | 0.43              |
| 46:CM:598:U:H2'    | 46:CM:599:A:H8     | 1.83                     | 0.43              |
| 46:CM:600:U:H2'    | 46:CM:601:U:C6     | 2.53                     | 0.43              |
| 46:CM:1648:U:H2'   | 46:CM:1649:G:H8    | 1.83                     | 0.43              |
| 47:CN:50:ILE:HA    | 47:CN:53:THR:HB    | 1.99                     | 0.43              |
| 47:CN:63:ILE:CD1   | 47:CN:158:VAL:HG21 | 2.48                     | 0.43              |
| 50:CQ:183:LEU:HD23 | 50:CQ:183:LEU:H    | 1.82                     | 0.43              |
| 51:CR:176:ASP:OD1  | 51:CR:177:THR:N    | 2.49                     | 0.43              |
| 54:CU:25:GLU:HB3   | 54:CU:31:LYS:HD2   | 1.99                     | 0.43              |
| 59:CZ:73:LYS:HB2   | 78:DS:150:VAL:HG11 | 2.00                     | 0.43              |
| 63:DD:12:LYS:HD2   | 63:DD:12:LYS:HA    | 1.90                     | 0.43              |
| 72:DM:80:LEU:HB3   | 72:DM:101:TYR:CE2  | 2.53                     | 0.43              |
| 79:DT:160:SER:C    | 79:DT:162:GLN:N    | 2.75                     | 0.43              |
| 1:1:152:U:O2'      | 1:1:153:U:H5'      | 2.18                     | 0.43              |
| 1:1:214:G:OP1      | 27:9:12:ARG:NH1    | 2.49                     | 0.43              |
| 1:1:409:A:H2       | 1:1:1437:G:N3      | 2.16                     | 0.43              |
| 1:1:411:U:H2'      | 1:1:412:G:H8       | 1.82                     | 0.43              |
| 1:1:1467:U:P       | 20:z:5:ARG:HH21    | 2.41                     | 0.43              |
| 1:1:1656:C:H2'     | 1:1:1657:G:H8      | 1.83                     | 0.43              |
| 1:1:1857:G:H1'     | 1:1:3038:U:H5''    | 2.00                     | 0.43              |
| 1:1:2482:U:H2'     | 1:1:2483:U:H5'     | 2.00                     | 0.43              |
| 3:4:131:G:H4'      | 26:8:93:HIS:ND1    | 2.33                     | 0.43              |
| 4:j:224:THR:HG22   | 4:j:240:ALA:HB3    | 1.99                     | 0.43              |
| 20:z:169:ALA:HA    | 20:z:172:ARG:CZ    | 2.48                     | 0.43              |
| 25:7:97:LYS:HG2    | 25:7:99:SER:H      | 1.82                     | 0.43              |
| 39:AL:31:VAL:HG23  | 39:AL:36:LYS:C     | 2.43                     | 0.43              |
| 46:B:194:G:H2'     | 46:B:195:A:O4'     | 2.19                     | 0.43              |
| 46:B:269:A:C2      | 46:B:283:G:C6      | 3.06                     | 0.43              |
| 46:B:687:A:C2      | 46:B:688:G:C4      | 3.06                     | 0.43              |
| 46:B:944:U:H5''    | 60:P:14:SER:HB3    | 2.00                     | 0.43              |
| 46:B:1092:G:O2'    | 46:B:1093:G:H5'    | 2.19                     | 0.43              |
| 51:G:118:GLU:HA    | 51:G:121:TYR:HE1   | 1.82                     | 0.43              |
| 51:G:173:ILE:HD11  | 51:G:236:TRP:CE2   | 2.53                     | 0.43              |
| 56:L:60:LEU:HD23   | 56:L:60:LEU:HA     | 1.86                     | 0.43              |
| 63:S:28:ILE:HA     | 63:S:64:ILE:O      | 2.18                     | 0.43              |
| 63:S:97:ASP:OD2    | 63:S:99:ALA:HB3    | 2.18                     | 0.43              |
| 79:AR:202:SER:C    | 79:AR:204:ASP:H    | 2.26                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AS:169:G:N1     | 1:AS:249:G:H1'     | 2.33                     | 0.43              |
| 1:AS:229:C:H2'    | 1:AS:230:G:O4'     | 2.17                     | 0.43              |
| 1:AS:359:U:H4'    | 1:AS:813:A:H62     | 1.83                     | 0.43              |
| 1:AS:1166:A:OP1   | 9:BB:215:ARG:HA    | 2.18                     | 0.43              |
| 1:AS:1440:G:H2'   | 1:AS:1441:U:O4'    | 2.18                     | 0.43              |
| 1:AS:2498:A:H2'   | 1:AS:2499:U:C6     | 2.53                     | 0.43              |
| 1:AS:2913:A:N7    | 5:AX:256:HIS:HE1   | 2.16                     | 0.43              |
| 1:AS:3196:U:H2'   | 1:AS:3197:G:C8     | 2.51                     | 0.43              |
| 1:AS:3262:U:H2'   | 1:AS:3263:C:H6     | 1.84                     | 0.43              |
| 3:AU:40:A:H2'     | 3:AU:41:A:H8       | 1.83                     | 0.43              |
| 3:AU:95:G:O2'     | 38:CE:81:GLY:O     | 2.25                     | 0.43              |
| 9:BB:108:GLN:HG2  | 9:BB:109:ILE:N     | 2.33                     | 0.43              |
| 16:BI:45:PRO:O    | 16:BI:49:ARG:HG3   | 2.19                     | 0.43              |
| 20:BM:151:ARG:O   | 20:BM:155:LEU:HD13 | 2.17                     | 0.43              |
| 29:BV:13:GLY:O    | 33:BZ:37:LYS:HD2   | 2.18                     | 0.43              |
| 43:CJ:93:LEU:HD12 | 43:CJ:93:LEU:HA    | 1.92                     | 0.43              |
| 46:CM:604:A:H4'   | 46:CM:605:G:H3'    | 2.00                     | 0.43              |
| 46:CM:739:A:H5''  | 46:CM:740:A:H5'    | 1.99                     | 0.43              |
| 46:CM:982:G:C6    | 46:CM:993:G:C6     | 3.06                     | 0.43              |
| 46:CM:1148:A:H2'  | 46:CM:1149:G:O4'   | 2.17                     | 0.43              |
| 46:CM:1315:G:H2'  | 46:CM:1316:A:C8    | 2.53                     | 0.43              |
| 52:CS:174:LEU:HB3 | 52:CS:210:ALA:CB   | 2.48                     | 0.43              |
| 53:CT:180:THR:H   | 53:CT:183:THR:HB   | 1.83                     | 0.43              |
| 71:DL:57:VAL:HB   | 71:DL:60:PHE:CE1   | 2.54                     | 0.43              |
| 72:DM:46:LYS:NZ   | 72:DM:69:LEU:O     | 2.41                     | 0.43              |
| 75:DP:60:GLU:H    | 75:DP:60:GLU:CD    | 2.25                     | 0.43              |
| 79:DT:16:HIS:NE2  | 79:DT:20:VAL:HG13  | 2.33                     | 0.43              |
| 79:DT:69:VAL:HG22 | 79:DT:85:SER:HB2   | 2.01                     | 0.43              |
| 79:DT:88:ARG:HA   | 79:DT:111:VAL:HG23 | 2.00                     | 0.43              |
| 1:1:600:U:H6      | 1:1:600:U:H2'      | 1.37                     | 0.43              |
| 1:1:640:U:O5'     | 1:1:640:U:H6       | 2.02                     | 0.43              |
| 1:1:1079:G:H2'    | 1:1:1080:A:C8      | 2.54                     | 0.43              |
| 1:1:1518:U:O2'    | 26:8:113:LEU:HD11  | 2.18                     | 0.43              |
| 1:1:1814:U:HO2'   | 1:1:1815:U:C5'     | 2.31                     | 0.43              |
| 1:1:2093:G:H22    | 1:1:2098:A:H1'     | 1.82                     | 0.43              |
| 1:1:2269:A:H2'    | 1:1:2270:U:C6      | 2.54                     | 0.43              |
| 1:1:2326:A:O2'    | 1:1:2369:G:OP1     | 2.24                     | 0.43              |
| 1:1:2351:A:N3     | 1:1:2796:G:O2'     | 2.37                     | 0.43              |
| 1:1:2438:U:H6     | 1:1:2438:U:H2'     | 1.67                     | 0.43              |
| 1:1:2465:U:H4'    | 1:1:2466:A:OP2     | 2.18                     | 0.43              |
| 1:1:2504:C:H2'    | 1:1:2505:G:C8      | 2.53                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:2581:A:H2'    | 1:1:2582:G:H8      | 1.83                     | 0.43              |
| 3:4:40:A:H2'      | 3:4:41:A:C8        | 2.52                     | 0.43              |
| 5:k:143:GLN:O     | 5:k:147:GLU:HG2    | 2.18                     | 0.43              |
| 11:q:42:ASP:HB2   | 11:q:64:HIS:NE2    | 2.34                     | 0.43              |
| 45:i:115:LEU:O    | 45:i:116:GLU:C     | 2.62                     | 0.43              |
| 46:B:299:A:H2'    | 46:B:300:U:C6      | 2.53                     | 0.43              |
| 46:B:674:C:H6     | 46:B:674:C:O5'     | 2.02                     | 0.43              |
| 46:B:1238:U:C2    | 46:B:1239:U:C5     | 3.07                     | 0.43              |
| 46:B:1305:U:O2    | 46:B:1307:A:H5'    | 2.18                     | 0.43              |
| 46:B:1341:U:H2'   | 46:B:1342:A:C8     | 2.54                     | 0.43              |
| 46:B:1584:A:C8    | 76:f:14:PHE:HD1    | 2.36                     | 0.43              |
| 49:E:138:TYR:CD1  | 49:E:142:ASN:HA    | 2.54                     | 0.43              |
| 50:F:73:LEU:CD2   | 57:M:20:VAL:HB     | 2.48                     | 0.43              |
| 50:F:102:GLN:OE1  | 50:F:123:VAL:HG23  | 2.19                     | 0.43              |
| 53:I:64:LYS:HB2   | 53:I:97:VAL:HG21   | 2.01                     | 0.43              |
| 55:K:103:GLN:HB3  | 55:K:170:ARG:HD3   | 2.00                     | 0.43              |
| 57:M:56:LYS:HZ2   | 57:M:69:THR:HG22   | 1.82                     | 0.43              |
| 57:M:77:ARG:CZ    | 57:M:86:ILE:HG22   | 2.48                     | 0.43              |
| 60:P:46:THR:C     | 60:P:50:ILE:HD12   | 2.43                     | 0.43              |
| 63:S:30:ILE:CG1   | 63:S:35:ILE:HG22   | 2.47                     | 0.43              |
| 1:AS:275:U:H2'    | 1:AS:276:U:C6      | 2.53                     | 0.43              |
| 1:AS:430:G:H2'    | 1:AS:431:A:C8      | 2.53                     | 0.43              |
| 1:AS:588:G:C2     | 1:AS:608:G:H2'     | 2.53                     | 0.43              |
| 1:AS:1014:G:H2'   | 1:AS:1015:G:C8     | 2.53                     | 0.43              |
| 1:AS:1099:A:H62   | 1:AS:1338:G:N2     | 2.17                     | 0.43              |
| 1:AS:2096:C:H2'   | 1:AS:2097:A:O4'    | 2.18                     | 0.43              |
| 1:AS:2242:U:H2'   | 1:AS:2243:C:C6     | 2.54                     | 0.43              |
| 1:AS:2749:G:H5''  | 1:AS:2750:G:OP1    | 2.17                     | 0.43              |
| 1:AS:2827:U:OP2   | 80:BE:6:ALA:HB3    | 2.19                     | 0.43              |
| 1:AS:3110:U:OP2   | 5:AX:30:LYS:HG3    | 2.18                     | 0.43              |
| 10:BC:227:TYR:CZ  | 10:BC:231:ARG:HD2  | 2.54                     | 0.43              |
| 14:BG:198:GLU:HA  | 14:BG:201:LYS:HG3  | 2.01                     | 0.43              |
| 18:BK:47:TYR:OH   | 18:BK:58:ILE:HD13  | 2.18                     | 0.43              |
| 24:BQ:42:THR:HG21 | 24:BQ:50:PRO:HG3   | 2.01                     | 0.43              |
| 25:BR:6:ASP:HB3   | 25:BR:10:GLY:H     | 1.83                     | 0.43              |
| 26:BS:74:LYS:HA   | 26:BS:77:GLU:CG    | 2.48                     | 0.43              |
| 28:BU:68:VAL:O    | 28:BU:115:LYS:HE2  | 2.17                     | 0.43              |
| 46:CM:66:U:H1'    | 53:CT:160:ARG:HH21 | 1.84                     | 0.43              |
| 46:CM:565:A:H5''  | 70:DK:70:LYS:NZ    | 2.33                     | 0.43              |
| 46:CM:823:G:H4'   | 46:CM:824:U:OP2    | 2.18                     | 0.43              |
| 47:CN:92:HIS:ND1  | 47:CN:202:TYR:OH   | 2.40                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:CR:88:ASP:OD1  | 51:CR:122:LYS:NZ   | 2.51                     | 0.43              |
| 55:CV:4:SER:OG    | 55:CV:6:ASP:OD1    | 2.34                     | 0.43              |
| 56:CW:88:GLU:OE1  | 56:CW:88:GLU:N     | 2.51                     | 0.43              |
| 59:CZ:40:GLY:HA2  | 59:CZ:124:LYS:HB2  | 2.01                     | 0.43              |
| 62:DC:75:VAL:HG22 | 62:DC:93:VAL:CG1   | 2.48                     | 0.43              |
| 65:DF:20:THR:HG21 | 65:DF:35:ILE:HA    | 2.00                     | 0.43              |
| 76:DQ:39:CYS:HB3  | 76:DQ:42:CYS:HB2   | 2.00                     | 0.43              |
| 79:DT:201:LEU:O   | 79:DT:201:LEU:HG   | 2.18                     | 0.43              |
| 81:P0:11:TYR:HE2  | 81:P0:59:VAL:HG22  | 1.82                     | 0.43              |
| 1:1:322:U:OP1     | 16:v:156:HIS:NE2   | 2.50                     | 0.43              |
| 1:1:798:C:C2      | 1:1:799:C:C5       | 3.06                     | 0.43              |
| 1:1:1165:A:H2'    | 1:1:1166:A:C8      | 2.53                     | 0.43              |
| 1:1:1513:A:OP1    | 40:AM:22:PRO:HG3   | 2.19                     | 0.43              |
| 1:1:1738:U:H6     | 1:1:1738:U:O5'     | 2.00                     | 0.43              |
| 1:1:2093:G:H4'    | 20:z:79:GLY:O      | 2.18                     | 0.43              |
| 1:1:2871:C:O2'    | 1:1:2873:G:OP2     | 2.23                     | 0.43              |
| 1:1:2876:U:H2'    | 1:1:2877:U:H6      | 1.83                     | 0.43              |
| 5:k:369:ARG:NH1   | 25:7:11:SER:OG     | 2.51                     | 0.43              |
| 6:l:272:LYS:HB2   | 6:l:275:TYR:HB3    | 2.00                     | 0.43              |
| 10:p:177:PRO:HG2  | 10:p:216:ILE:HD13  | 2.01                     | 0.43              |
| 25:7:13:ILE:HD12  | 25:7:30:ARG:HB3    | 2.01                     | 0.43              |
| 46:B:744:U:N3     | 46:B:745:A:N7      | 2.67                     | 0.43              |
| 46:B:1670:U:H3    | 46:B:1705:G:H1     | 1.67                     | 0.43              |
| 47:C:55:GLU:HB3   | 68:X:79:LEU:HD22   | 2.00                     | 0.43              |
| 48:D:131:ASP:OD2  | 48:D:180:THR:OG1   | 2.36                     | 0.43              |
| 53:I:121:ILE:HB   | 53:I:124:LEU:HB3   | 2.00                     | 0.43              |
| 53:I:149:LYS:HE2  | 53:I:149:LYS:HB3   | 1.72                     | 0.43              |
| 66:V:108:LEU:HD12 | 66:V:108:LEU:HA    | 1.80                     | 0.43              |
| 76:f:20:GLN:HA    | 76:f:26:SER:O      | 2.18                     | 0.43              |
| 1:AS:291:C:H2'    | 1:AS:292:U:H6      | 1.83                     | 0.43              |
| 1:AS:648:C:H2'    | 1:AS:649:G:C8      | 2.53                     | 0.43              |
| 1:AS:987:G:C6     | 1:AS:1055:G:C6     | 3.07                     | 0.43              |
| 1:AS:1043:A:H2'   | 1:AS:1044:A:C8     | 2.54                     | 0.43              |
| 1:AS:1905:A:O5'   | 1:AS:1905:A:H8     | 2.00                     | 0.43              |
| 1:AS:2192:A:H2'   | 1:AS:2193:A:O4'    | 2.19                     | 0.43              |
| 13:BF:52:TYR:CD1  | 45:CL:47:ASP:HB3   | 2.54                     | 0.43              |
| 14:BG:159:ARG:HB3 | 29:BV:124:ILE:HD12 | 1.99                     | 0.43              |
| 19:BL:176:ARG:N   | 29:BV:51:GLY:HA2   | 2.33                     | 0.43              |
| 23:BP:35:LYS:O    | 23:BP:39:GLU:HG3   | 2.18                     | 0.43              |
| 23:BP:52:ASN:O    | 23:BP:53:ASP:C     | 2.62                     | 0.43              |
| 27:BT:39:LEU:HD12 | 27:BT:106:ILE:O    | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BT:43:TYR:HA    | 27:BT:125:LYS:O    | 2.17                     | 0.43              |
| 35:CB:30:LEU:HD12  | 35:CB:30:LEU:HA    | 1.90                     | 0.43              |
| 46:CM:1332:U:C4    | 67:DH:57:MET:HE1   | 2.53                     | 0.43              |
| 46:CM:1378:U:H2'   | 46:CM:1379:C:C6    | 2.53                     | 0.43              |
| 46:CM:1401:U:H5''  | 64:DE:3:ARG:HH21   | 1.83                     | 0.43              |
| 46:CM:1444:G:OP1   | 65:DF:138:THR:N    | 2.48                     | 0.43              |
| 51:CR:163:ASP:C    | 51:CR:165:ALA:H    | 2.27                     | 0.43              |
| 52:CS:161:ASP:O    | 75:DP:44:VAL:HA    | 2.18                     | 0.43              |
| 53:CT:2:LYS:O      | 53:CT:108:VAL:HA   | 2.18                     | 0.43              |
| 53:CT:56:ASN:HB2   | 53:CT:108:VAL:HG12 | 1.99                     | 0.43              |
| 53:CT:137:ARG:O    | 53:CT:141:ILE:HG13 | 2.18                     | 0.43              |
| 54:CU:42:ILE:HA    | 54:CU:55:ALA:O     | 2.18                     | 0.43              |
| 54:CU:104:LYS:HE3  | 54:CU:104:LYS:HB3  | 1.76                     | 0.43              |
| 54:CU:169:TYR:HE2  | 54:CU:175:LYS:HB2  | 1.82                     | 0.43              |
| 55:CV:60:VAL:HG21  | 55:CV:185:CYS:SG   | 2.58                     | 0.43              |
| 56:CW:34:TYR:CD2   | 56:CW:105:LEU:HD22 | 2.53                     | 0.43              |
| 62:DC:20:VAL:HG21  | 62:DC:36:LEU:CD1   | 2.42                     | 0.43              |
| 66:DG:86:ARG:NH1   | 66:DG:90:PRO:O     | 2.37                     | 0.43              |
| 79:DT:7:LEU:O      | 79:DT:310:TRP:HB3  | 2.17                     | 0.43              |
| 79:DT:289:LEU:HD23 | 79:DT:289:LEU:H    | 1.83                     | 0.43              |
| 1:1:14:C:H2'       | 1:1:15:A:C8        | 2.53                     | 0.43              |
| 1:1:154:G:H5''     | 1:1:155:A:H2'      | 2.01                     | 0.43              |
| 1:1:210:A:OP2      | 6:l:222:ASN:HB2    | 2.18                     | 0.43              |
| 1:1:928:U:O4'      | 1:1:930:G:H5'      | 2.19                     | 0.43              |
| 1:1:1467:U:H2'     | 1:1:1468:U:C6      | 2.54                     | 0.43              |
| 1:1:1589:A:N3      | 1:1:1611:U:O2'     | 2.49                     | 0.43              |
| 1:1:2079:C:O2'     | 1:1:2080:U:H6      | 2.01                     | 0.43              |
| 1:1:2094:G:OP1     | 1:1:2096:C:N4      | 2.49                     | 0.43              |
| 1:1:2698:C:O2'     | 1:1:2699:A:H2'     | 2.19                     | 0.43              |
| 1:1:3024:G:H2'     | 1:1:3025:G:H8      | 1.83                     | 0.43              |
| 1:1:3122:A:H5'     | 5:k:130:PHE:H      | 1.84                     | 0.43              |
| 6:l:303:ALA:CB     | 19:y:39:ARG:HH12   | 2.27                     | 0.43              |
| 14:t:80:LEU:HD11   | 14:t:97:VAL:HG22   | 2.01                     | 0.43              |
| 16:v:65:ARG:HG2    | 16:v:127:TYR:CD1   | 2.53                     | 0.43              |
| 17:w:126:ARG:HG2   | 17:w:130:LEU:HD12  | 2.01                     | 0.43              |
| 19:y:40:THR:C      | 19:y:42:ALA:H      | 2.26                     | 0.43              |
| 33:AF:10:ILE:HA    | 33:AF:64:THR:HG21  | 2.01                     | 0.43              |
| 46:B:280:C:H2'     | 46:B:281:U:O4'     | 2.18                     | 0.43              |
| 46:B:1532:A:H2'    | 46:B:1533:G:H8     | 1.83                     | 0.43              |
| 46:B:1597:G:N7     | 63:S:13:LYS:NZ     | 2.67                     | 0.43              |
| 47:C:205:ARG:HD3   | 64:T:84:TYR:HD2    | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:K:107:THR:OG1  | 55:K:108:PRO:HD3  | 2.19                     | 0.43              |
| 69:Y:11:LEU:HD12  | 69:Y:74:VAL:HG13  | 2.00                     | 0.43              |
| 79:AR:132:VAL:O   | 79:AR:145:LEU:HB2 | 2.19                     | 0.43              |
| 1:AS:844:A:N6     | 1:AS:845:C:O2     | 2.52                     | 0.43              |
| 1:AS:856:G:O2'    | 1:AS:891:A:H4'    | 2.19                     | 0.43              |
| 1:AS:1556:G:O2'   | 1:AS:1557:U:H5'   | 2.19                     | 0.43              |
| 1:AS:1634:A:OP1   | 35:CB:74:ARG:NH1  | 2.52                     | 0.43              |
| 1:AS:2484:U:C2    | 1:AS:2485:U:C5    | 3.07                     | 0.43              |
| 1:AS:2564:G:H4'   | 1:AS:2566:C:C2    | 2.53                     | 0.43              |
| 1:AS:2718:A:H2'   | 1:AS:2719:A:O4'   | 2.18                     | 0.43              |
| 1:AS:2957:C:H2'   | 1:AS:2958:U:C6    | 2.53                     | 0.43              |
| 1:AS:3336:G:H2'   | 1:AS:3337:A:H8    | 1.83                     | 0.43              |
| 3:AU:24:G:H2'     | 3:AU:25:G:O4'     | 2.18                     | 0.43              |
| 7:AZ:60:ILE:H     | 7:AZ:80:ALA:CB    | 2.31                     | 0.43              |
| 10:BC:154:ILE:O   | 10:BC:180:ILE:HA  | 2.19                     | 0.43              |
| 14:BG:85:ILE:HG23 | 14:BG:89:TYR:HD2  | 1.82                     | 0.43              |
| 21:BN:83:SER:OG   | 21:BN:88:HIS:NE2  | 2.44                     | 0.43              |
| 24:BQ:14:SER:H    | 24:BQ:85:TRP:HB2  | 1.84                     | 0.43              |
| 29:BV:119:PRO:O   | 29:BV:121:VAL:N   | 2.51                     | 0.43              |
| 35:CB:57:LEU:HB2  | 35:CB:62:TYR:HE1  | 1.79                     | 0.43              |
| 46:CM:810:U:H2'   | 46:CM:811:U:C6    | 2.54                     | 0.43              |
| 46:CM:872:A:H2'   | 46:CM:873:U:H6    | 1.83                     | 0.43              |
| 46:CM:872:A:C1'   | 61:DB:117:PRO:HB3 | 2.48                     | 0.43              |
| 46:CM:1132:A:H2'  | 46:CM:1133:C:C6   | 2.54                     | 0.43              |
| 46:CM:1445:C:N4   | 65:DF:139:LYS:HG3 | 2.34                     | 0.43              |
| 46:CM:1636:C:H2'  | 46:CM:1637:U:H6   | 1.84                     | 0.43              |
| 46:CM:1647:A:H2'  | 46:CM:1648:U:C6   | 2.54                     | 0.43              |
| 46:CM:1721:U:H2'  | 46:CM:1722:U:C6   | 2.52                     | 0.43              |
| 60:DA:83:GLU:OE1  | 60:DA:83:GLU:N    | 2.50                     | 0.43              |
| 61:DB:88:THR:HA   | 61:DB:89:PRO:HD3  | 1.90                     | 0.43              |
| 62:DC:55:GLY:O    | 62:DC:59:LYS:HG3  | 2.18                     | 0.43              |
| 63:DD:31:ASN:OD1  | 63:DD:67:LYS:HA   | 2.19                     | 0.43              |
| 66:DG:103:LYS:HA  | 66:DG:103:LYS:HD3 | 1.75                     | 0.43              |
| 70:DK:92:CYS:HA   | 70:DK:95:PHE:HD2  | 1.84                     | 0.43              |
| 79:DT:73:THR:HG22 | 79:DT:74:ILE:O    | 2.18                     | 0.43              |
| 79:DT:189:PHE:HB3 | 79:DT:220:TRP:CZ2 | 2.53                     | 0.43              |
| 79:DT:243:SER:HB3 | 79:DT:248:TRP:N   | 2.21                     | 0.43              |
| 82:12:104:ILE:N   | 82:12:105:PRO:CD  | 2.80                     | 0.43              |
| 1:1:14:C:H2'      | 1:1:15:A:H8       | 1.83                     | 0.43              |
| 1:1:225:C:H2'     | 1:1:226:G:O4'     | 2.18                     | 0.43              |
| 1:1:352:A:N1      | 1:1:365:A:H5''    | 2.34                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:1:495:C:H2'     | 1:1:496:A:H8     | 1.83                     | 0.43              |
| 1:1:591:C:OP2     | 8:n:18:LYS:HG2   | 2.18                     | 0.43              |
| 1:1:655:A:H2'     | 1:1:656:G:H8     | 1.84                     | 0.43              |
| 1:1:872:A:H5''    | 1:1:1886:U:H5''  | 2.00                     | 0.43              |
| 1:1:2339:A:H2'    | 1:1:2340:C:C6    | 2.53                     | 0.43              |
| 1:1:2510:U:H2'    | 1:1:2511:G:C8    | 2.54                     | 0.43              |
| 1:1:2516:U:C3'    | 1:1:2519:A:H61   | 2.32                     | 0.43              |
| 1:1:3157:A:N1     | 21:0:171:PHE:HB3 | 2.33                     | 0.43              |
| 1:1:3199:G:H2'    | 1:1:3200:C:C6    | 2.54                     | 0.43              |
| 6:l:113:LYS:HE3   | 16:v:202:TYR:HB3 | 2.01                     | 0.43              |
| 13:s:61:ARG:NH1   | 45:i:44:ALA:O    | 2.37                     | 0.43              |
| 19:y:76:ALA:HA    | 19:y:79:LYS:HG3  | 2.00                     | 0.43              |
| 19:y:165:ILE:HD11 | 19:y:172:PHE:HB3 | 2.00                     | 0.43              |
| 21:0:40:ARG:HD2   | 21:0:40:ARG:HA   | 1.70                     | 0.43              |
| 27:9:86:GLN:HB3   | 27:9:94:SER:HB3  | 2.00                     | 0.43              |
| 45:i:69:PHE:HB2   | 65:U:129:TRP:NE1 | 2.34                     | 0.43              |
| 46:B:382:G:H2'    | 46:B:383:A:C8    | 2.54                     | 0.43              |
| 46:B:814:A:H2     | 46:B:815:U:H3    | 1.65                     | 0.43              |
| 46:B:944:U:OP2    | 74:d:20:LYS:NZ   | 2.52                     | 0.43              |
| 46:B:964:A:H4'    | 46:B:1773:G:N2   | 2.33                     | 0.43              |
| 46:B:1163:G:H5'   | 46:B:1175:C:H42  | 1.84                     | 0.43              |
| 46:B:1457:A:H2    | 46:B:1460:G:N3   | 2.17                     | 0.43              |
| 47:C:49:ASN:HD22  | 47:C:52:LYS:HE3  | 1.81                     | 0.43              |
| 50:F:72:SER:O     | 50:F:75:VAL:HG22 | 2.18                     | 0.43              |
| 50:F:125:ARG:HD3  | 50:F:125:ARG:HA  | 1.70                     | 0.43              |
| 51:G:194:VAL:HG11 | 51:G:232:ALA:HB2 | 2.01                     | 0.43              |
| 53:I:76:LEU:HB2   | 53:I:94:ARG:NH1  | 2.33                     | 0.43              |
| 61:Q:20:ASP:OD1   | 61:Q:21:THR:N    | 2.45                     | 0.43              |
| 61:Q:82:GLY:HA3   | 61:Q:115:PRO:HG2 | 2.00                     | 0.43              |
| 62:R:1:MET:HB3    | 65:U:18:LEU:H    | 1.83                     | 0.43              |
| 62:R:80:LEU:HD12  | 62:R:80:LEU:O    | 2.18                     | 0.43              |
| 63:S:131:ARG:HG3  | 63:S:137:PHE:CE1 | 2.51                     | 0.43              |
| 1:AS:821:U:H5''   | 1:AS:1793:A:C5   | 2.53                     | 0.43              |
| 1:AS:1011:C:H4'   | 1:AS:1012:U:C6   | 2.49                     | 0.43              |
| 1:AS:1400:G:N1    | 1:AS:1404:A:C6   | 2.87                     | 0.43              |
| 1:AS:1466:U:H2'   | 1:AS:1467:U:C6   | 2.54                     | 0.43              |
| 1:AS:1706:C:H2'   | 1:AS:1707:U:C6   | 2.54                     | 0.43              |
| 1:AS:2143:G:OP1   | 16:BI:77:LYS:HE3 | 2.18                     | 0.43              |
| 1:AS:2583:U:H2'   | 1:AS:2584:U:C6   | 2.53                     | 0.43              |
| 1:AS:2814:U:O2    | 1:AS:2814:U:H2'  | 2.19                     | 0.43              |
| 1:AS:2969:G:C6    | 1:AS:3361:U:C4   | 3.07                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AS:3179:U:C6    | 15:BH:114:MET:HE1  | 2.54                     | 0.43              |
| 3:AU:8:C:H2'      | 3:AU:9:A:C8        | 2.52                     | 0.43              |
| 3:AU:22:U:H5''    | 27:BT:16:ARG:HH12  | 1.84                     | 0.43              |
| 14:BG:134:GLU:O   | 14:BG:137:SER:OG   | 2.26                     | 0.43              |
| 26:BS:109:TYR:CE1 | 26:BS:125:ARG:HB3  | 2.54                     | 0.43              |
| 26:BS:115:ARG:O   | 26:BS:117:ASN:N    | 2.48                     | 0.43              |
| 28:BU:22:LYS:HD3  | 28:BU:129:TRP:CZ3  | 2.54                     | 0.43              |
| 28:BU:57:MET:HB3  | 28:BU:61:LYS:HE2   | 1.99                     | 0.43              |
| 40:CG:23:LEU:HD12 | 40:CG:24:PRO:HD2   | 2.00                     | 0.43              |
| 45:CL:82:LYS:HA   | 45:CL:82:LYS:HD2   | 1.58                     | 0.43              |
| 46:CM:121:U:H1'   | 51:CR:33:ALA:HB3   | 2.01                     | 0.43              |
| 46:CM:641:G:O6    | 46:CM:690:C:N4     | 2.52                     | 0.43              |
| 46:CM:907:G:H2'   | 46:CM:908:A:C8     | 2.54                     | 0.43              |
| 46:CM:921:G:O6    | 73:DN:15:ARG:HD3   | 2.19                     | 0.43              |
| 46:CM:1030:C:H2'  | 46:CM:1031:G:H8    | 1.83                     | 0.43              |
| 46:CM:1487:C:OP1  | 66:DG:122:ARG:NH2  | 2.47                     | 0.43              |
| 46:CM:1546:G:C5   | 65:DF:134:ARG:HD3  | 2.53                     | 0.43              |
| 53:CT:104:GLN:OE1 | 53:CT:104:GLN:N    | 2.51                     | 0.43              |
| 54:CU:11:THR:O    | 54:CU:15:LEU:HD12  | 2.17                     | 0.43              |
| 54:CU:12:GLU:CD   | 54:CU:16:LYS:HD3   | 2.44                     | 0.43              |
| 54:CU:46:ASP:CG   | 54:CU:52:LYS:HG2   | 2.44                     | 0.43              |
| 57:CX:25:LYS:HD2  | 57:CX:59:PHE:HZ    | 1.84                     | 0.43              |
| 59:CZ:116:VAL:O   | 59:CZ:117:GLY:C    | 2.61                     | 0.43              |
| 59:CZ:137:LEU:HA  | 59:CZ:140:PHE:CZ   | 2.53                     | 0.43              |
| 64:DE:74:GLN:O    | 64:DE:78:ARG:HB3   | 2.19                     | 0.43              |
| 79:DT:16:HIS:HB3  | 79:DT:305:ASN:O    | 2.19                     | 0.43              |
| 79:DT:238:HIS:CD2 | 79:DT:287:ILE:HG22 | 2.53                     | 0.43              |
| 81:P0:16:ARG:CD   | 81:P0:66:PHE:CE2   | 3.01                     | 0.43              |
| 82:12:105:PRO:CD  | 82:12:106:LEU:H    | 2.29                     | 0.43              |
| 82:12:118:HIS:ND1 | 82:12:119:LYS:HD3  | 2.33                     | 0.43              |
| 1:1:163:A:H2'     | 1:1:164:U:C1'      | 2.49                     | 0.43              |
| 1:1:275:U:H2'     | 1:1:276:U:C6       | 2.54                     | 0.43              |
| 1:1:290:G:H2'     | 1:1:291:C:C6       | 2.54                     | 0.43              |
| 1:1:364:G:OP1     | 6:l:61:THR:HG23    | 2.18                     | 0.43              |
| 1:1:437:G:O2'     | 1:1:438:A:H5''     | 2.19                     | 0.43              |
| 1:1:532:U:OP1     | 21:0:146:LYS:NZ    | 2.23                     | 0.43              |
| 1:1:698:C:H2'     | 1:1:699:G:C8       | 2.53                     | 0.43              |
| 1:1:1761:U:C6     | 20:z:43:LYS:HE3    | 2.54                     | 0.43              |
| 1:1:1852:C:H2'    | 1:1:1853:C:C6      | 2.51                     | 0.43              |
| 1:1:1883:A:H5'    | 5:k:226:PHE:O      | 2.19                     | 0.43              |
| 1:1:2221:A:H3'    | 4:j:244:GLY:HA2    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:3190:C:C2     | 1:1:3191:A:C8      | 3.07                     | 0.43              |
| 1:1:3264:C:C2     | 1:1:3265:U:C5      | 3.06                     | 0.43              |
| 3:4:2:A:C4        | 3:4:3:A:C8         | 3.07                     | 0.43              |
| 3:4:13:A:C6       | 3:4:14:C:C4        | 3.07                     | 0.43              |
| 5:k:219:ALA:HB3   | 5:k:329:PRO:HG2    | 2.00                     | 0.43              |
| 7:m:290:ILE:HG12  | 12:r:210:LEU:HD11  | 2.00                     | 0.43              |
| 9:o:153:LYS:HG3   | 9:o:201:TRP:CZ3    | 2.54                     | 0.43              |
| 10:p:48:SER:HA    | 10:p:51:VAL:HG23   | 2.00                     | 0.43              |
| 11:q:10:LEU:HD21  | 11:q:79:ILE:CD1    | 2.49                     | 0.43              |
| 13:s:12:LEU:HD23  | 13:s:12:LEU:HA     | 1.88                     | 0.43              |
| 20:z:38:ARG:O     | 20:z:42:ARG:HG3    | 2.18                     | 0.43              |
| 26:8:81:THR:HA    | 26:8:125:ARG:HA    | 2.01                     | 0.43              |
| 39:AL:14:LEU:HD21 | 39:AL:52:TYR:CG    | 2.54                     | 0.43              |
| 46:B:138:C:O4'    | 53:I:179:VAL:HG11  | 2.19                     | 0.43              |
| 46:B:220:A:O5'    | 46:B:220:A:H8      | 2.02                     | 0.43              |
| 46:B:234:G:H8     | 46:B:234:G:O5'     | 2.02                     | 0.43              |
| 46:B:298:A:H2'    | 46:B:299:A:C8      | 2.54                     | 0.43              |
| 46:B:1141:C:H2'   | 46:B:1142:A:H8     | 1.84                     | 0.43              |
| 46:B:1389:U:H2'   | 46:B:1390:C:C6     | 2.54                     | 0.43              |
| 46:B:1740:A:N3    | 77:g:2:GLY:N       | 2.66                     | 0.43              |
| 48:D:88:VAL:HA    | 48:D:98:THR:HA     | 1.99                     | 0.43              |
| 54:J:122:LEU:HD11 | 54:J:148:VAL:HG21  | 2.01                     | 0.43              |
| 55:K:158:ILE:CD1  | 55:K:163:ASP:OD1   | 2.63                     | 0.43              |
| 58:N:132:SER:HB3  | 58:N:135:VAL:HB    | 2.00                     | 0.43              |
| 72:b:60:VAL:HG23  | 72:b:101:TYR:HB2   | 2.00                     | 0.43              |
| 1:AS:163:A:H2'    | 1:AS:164:U:O4'     | 2.18                     | 0.43              |
| 1:AS:1633:A:P     | 28:BU:73:LYS:HZ1   | 2.42                     | 0.43              |
| 1:AS:1714:G:H5''  | 20:BM:117:LYS:HG3  | 2.01                     | 0.43              |
| 1:AS:3152:G:H2'   | 1:AS:3153:A:C8     | 2.54                     | 0.43              |
| 1:AS:3165:U:N3    | 1:AS:3166:A:H1'    | 2.32                     | 0.43              |
| 1:AS:3199:G:H2'   | 1:AS:3200:C:H6     | 1.84                     | 0.43              |
| 3:AU:36:G:OP2     | 36:CC:85:THR:OG1   | 2.19                     | 0.43              |
| 5:AX:256:HIS:HA   | 5:AX:257:PRO:C     | 2.44                     | 0.43              |
| 7:AZ:95:TRP:HD1   | 7:AZ:158:ARG:HA    | 1.80                     | 0.43              |
| 18:BK:29:THR:HA   | 18:BK:32:THR:HG22  | 2.01                     | 0.43              |
| 19:BL:104:LEU:HA  | 19:BL:104:LEU:HD23 | 1.69                     | 0.43              |
| 29:BV:76:ASP:HB3  | 29:BV:116:GLY:HA3  | 2.01                     | 0.43              |
| 36:CC:49:LYS:O    | 36:CC:53:ARG:HG3   | 2.19                     | 0.43              |
| 37:CD:78:THR:HG22 | 37:CD:81:ARG:HG3   | 2.01                     | 0.43              |
| 39:CF:30:LYS:HG3  | 39:CF:31:VAL:H     | 1.83                     | 0.43              |
| 39:CF:38:PHE:CG   | 39:CF:39:LYS:N     | 2.87                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:CG:20:ASN:OD1   | 40:CG:42:ARG:HG2  | 2.19                     | 0.43              |
| 46:CM:261:C:O2'    | 46:CM:262:G:H5'   | 2.19                     | 0.43              |
| 46:CM:824:U:OP1    | 58:CY:27:ALA:HB3  | 2.19                     | 0.43              |
| 46:CM:883:A:H1'    | 46:CM:884:G:H1'   | 1.99                     | 0.43              |
| 46:CM:974:U:H2'    | 46:CM:975:C:C6    | 2.54                     | 0.43              |
| 46:CM:1370:A:H2'   | 46:CM:1371:G:O4'  | 2.19                     | 0.43              |
| 47:CN:43:ASP:OD1   | 47:CN:44:GLY:N    | 2.52                     | 0.43              |
| 48:CO:32:ILE:HG12  | 48:CO:44:GLY:O    | 2.18                     | 0.43              |
| 48:CO:70:LEU:CD2   | 48:CO:79:HIS:CD2  | 2.95                     | 0.43              |
| 53:CT:136:LYS:HE3  | 53:CT:174:LYS:O   | 2.19                     | 0.43              |
| 54:CU:86:VAL:O     | 54:CU:161:LYS:HE3 | 2.18                     | 0.43              |
| 55:CV:36:THR:HB    | 55:CV:96:LEU:O    | 2.19                     | 0.43              |
| 59:CZ:36:LEU:HB2   | 59:CZ:41:LEU:CG   | 2.38                     | 0.43              |
| 59:CZ:42:ALA:HB3   | 59:CZ:48:ALA:HA   | 2.00                     | 0.43              |
| 67:DH:70:PRO:HA    | 76:DQ:41:GLN:HG3  | 2.00                     | 0.43              |
| 78:DS:161:ARG:HH21 | 78:DS:163:CYS:H   | 1.67                     | 0.43              |
| 79:DT:67:HIS:CG    | 79:DT:86:TRP:HB2  | 2.53                     | 0.43              |
| 79:DT:110:ASP:O    | 79:DT:127:SER:HA  | 2.19                     | 0.43              |
| 79:DT:258:LYS:HB3  | 79:DT:260:PHE:CE1 | 2.54                     | 0.43              |
| 81:P0:55:LYS:CG    | 81:P0:56:ASN:N    | 2.82                     | 0.43              |
| 1:1:196:G:H2'      | 1:1:197:A:C8      | 2.54                     | 0.43              |
| 1:1:520:G:C4       | 1:1:521:G:C8      | 3.07                     | 0.43              |
| 1:1:629:A:H2'      | 1:1:630:G:C8      | 2.53                     | 0.43              |
| 1:1:1093:G:H5'     | 22:2:129:LYS:HE2  | 2.01                     | 0.43              |
| 1:1:2718:A:H2'     | 1:1:2719:A:O4'    | 2.19                     | 0.43              |
| 1:1:3128:G:C6      | 1:1:3129:C:C5     | 3.07                     | 0.43              |
| 2:3:77:G:H3'       | 21:0:46:GLN:O     | 2.19                     | 0.43              |
| 2:3:84:A:H2'       | 2:3:85:G:C8       | 2.54                     | 0.43              |
| 29:AB:119:PRO:O    | 29:AB:121:VAL:N   | 2.49                     | 0.43              |
| 44:AQ:47:VAL:HA    | 44:AQ:56:ASN:O    | 2.18                     | 0.43              |
| 46:B:562:G:O2'     | 46:B:575:G:H4'    | 2.19                     | 0.43              |
| 46:B:583:A:H2'     | 46:B:584:G:C8     | 2.54                     | 0.43              |
| 46:B:627:U:H2'     | 46:B:628:A:H8     | 1.84                     | 0.43              |
| 46:B:635:C:OP1     | 69:Y:32:LYS:HG3   | 2.19                     | 0.43              |
| 46:B:827:C:H5''    | 46:B:828:U:OP2    | 2.19                     | 0.43              |
| 46:B:1453:C:O2'    | 66:V:88:PHE:O     | 2.17                     | 0.43              |
| 52:H:139:ASN:O     | 52:H:214:LYS:HE2  | 2.18                     | 0.43              |
| 54:J:169:TYR:OH    | 54:J:175:LYS:HE3  | 2.19                     | 0.43              |
| 55:K:158:ILE:CG1   | 55:K:163:ASP:OD1  | 2.67                     | 0.43              |
| 64:T:90:ALA:HA     | 64:T:95:HIS:CD2   | 2.54                     | 0.43              |
| 70:Z:107:PHE:CD2   | 70:Z:114:LYS:HD3  | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:AR:12:THR:O     | 79:AR:53:ASN:HA    | 2.19                     | 0.43              |
| 1:AS:513:G:O2'     | 1:AS:514:G:H5'     | 2.19                     | 0.43              |
| 1:AS:605:U:C2      | 8:BA:25:ARG:NH1    | 2.87                     | 0.43              |
| 1:AS:643:A:H1'     | 1:AS:645:A:OP2     | 2.19                     | 0.43              |
| 1:AS:976:A:H8      | 1:AS:976:A:H3'     | 1.84                     | 0.43              |
| 1:AS:1424:A:OP2    | 29:BV:2:PRO:HA     | 2.19                     | 0.43              |
| 1:AS:2159:C:H5''   | 4:AW:193:ARG:CZ    | 2.49                     | 0.43              |
| 1:AS:2525:A:H2'    | 1:AS:2526:C:O4'    | 2.19                     | 0.43              |
| 1:AS:2660:U:O4     | 7:AZ:19:PRO:HD3    | 2.19                     | 0.43              |
| 1:AS:2869:A:H5''   | 41:CH:49:LYS:HB2   | 2.00                     | 0.43              |
| 1:AS:3204:G:H2'    | 1:AS:3205:C:H6     | 1.84                     | 0.43              |
| 3:AU:65:A:OP1      | 36:CC:53:ARG:NE    | 2.52                     | 0.43              |
| 3:AU:85:G:O6       | 27:BT:114:ASP:N    | 2.47                     | 0.43              |
| 4:AW:109:GLU:HG3   | 4:AW:138:GLY:HA2   | 2.00                     | 0.43              |
| 6:AY:258:SER:O     | 6:AY:262:VAL:HG23  | 2.18                     | 0.43              |
| 6:AY:345:VAL:HG11  | 9:BB:58:ARG:CZ     | 2.49                     | 0.43              |
| 10:BC:151:LEU:HD22 | 10:BC:216:ILE:CD1  | 2.49                     | 0.43              |
| 80:BE:42:THR:O     | 80:BE:139:ARG:NH2  | 2.50                     | 0.43              |
| 80:BE:86:HIS:HB3   | 80:BE:139:ARG:HG3  | 2.00                     | 0.43              |
| 13:BF:61:ARG:NH1   | 13:BF:62:ASN:OD1   | 2.52                     | 0.43              |
| 25:BR:111:LYS:NZ   | 53:CT:154:ARG:HH12 | 2.17                     | 0.43              |
| 26:BS:88:ILE:O     | 26:BS:120:LYS:NZ   | 2.49                     | 0.43              |
| 46:CM:103:A:O3'    | 46:CM:306:C:N4     | 2.52                     | 0.43              |
| 46:CM:233:G:H2'    | 46:CM:234:G:O4'    | 2.19                     | 0.43              |
| 46:CM:1215:A:H2    | 46:CM:1243:U:O2    | 2.02                     | 0.43              |
| 48:CO:33:LYS:N     | 48:CO:96:LEU:O     | 2.43                     | 0.43              |
| 59:CZ:97:LEU:HD22  | 59:CZ:119:SER:O    | 2.19                     | 0.43              |
| 59:CZ:132:GLU:HA   | 59:CZ:136:LEU:CD1  | 2.36                     | 0.43              |
| 68:DI:5:LYS:HD2    | 68:DI:7:GLN:HE22   | 1.83                     | 0.43              |
| 81:P0:66:PHE:CE2   | 81:P0:70:LEU:HD12  | 2.54                     | 0.43              |
| 1:1:143:A:H2'      | 1:1:144:G:O4'      | 2.18                     | 0.43              |
| 1:1:269:G:OP2      | 16:v:44:ARG:NH1    | 2.51                     | 0.43              |
| 1:1:426:G:H4'      | 33:AF:52:PRO:HD3   | 1.99                     | 0.43              |
| 1:1:2096:C:H2'     | 1:1:2097:A:O4'     | 2.19                     | 0.43              |
| 1:1:3056:C:O2'     | 1:1:3297:U:OP1     | 2.31                     | 0.43              |
| 1:1:3079:U:H2'     | 1:1:3080:G:H8      | 1.84                     | 0.43              |
| 4:j:201:GLY:O      | 4:j:204:MET:HG3    | 2.19                     | 0.43              |
| 6:l:84:HIS:ND1     | 6:l:84:HIS:O       | 2.52                     | 0.43              |
| 6:l:318:PRO:HG2    | 9:o:147:TYR:HB3    | 2.00                     | 0.43              |
| 7:m:85:ARG:NH2     | 7:m:250:ASP:OD2    | 2.51                     | 0.43              |
| 16:v:45:PRO:O      | 16:v:49:ARG:HG3    | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:AI:105:ARG:HG3  | 36:AI:108:ARG:HH21 | 1.84                     | 0.43              |
| 45:i:104:GLN:HG3   | 45:i:109:GLN:HE21  | 1.81                     | 0.43              |
| 46:B:45:U:O2       | 46:B:432:G:H1'     | 2.19                     | 0.43              |
| 46:B:52:U:H2'      | 46:B:53:G:H8       | 1.80                     | 0.43              |
| 46:B:97:C:H2'      | 46:B:98:U:C6       | 2.54                     | 0.43              |
| 46:B:444:A:H5''    | 51:G:57:ASN:HD22   | 1.83                     | 0.43              |
| 46:B:1545:U:H3     | 62:R:122:THR:HG22  | 1.83                     | 0.43              |
| 47:C:84:ARG:HD3    | 47:C:203:PHE:O     | 2.18                     | 0.43              |
| 50:F:76:LYS:NZ     | 57:M:18:GLU:HG2    | 2.34                     | 0.43              |
| 51:G:118:GLU:HA    | 51:G:121:TYR:CE1   | 2.53                     | 0.43              |
| 56:L:62:ARG:NH2    | 56:L:68:LYS:HD3    | 2.33                     | 0.43              |
| 58:N:2:ALA:HB2     | 58:N:116:ARG:HH11  | 1.84                     | 0.43              |
| 74:d:38:GLN:HB2    | 74:d:76:GLY:HA3    | 2.01                     | 0.43              |
| 1:AS:291:C:C2      | 1:AS:292:U:C5      | 3.06                     | 0.43              |
| 1:AS:561:U:H2'     | 1:AS:562:C:H6      | 1.83                     | 0.43              |
| 1:AS:1065:C:H2'    | 1:AS:1066:U:H6     | 1.83                     | 0.43              |
| 1:AS:1654:G:C5     | 1:AS:1792:G:C6     | 3.06                     | 0.43              |
| 1:AS:2181:U:H2'    | 1:AS:2182:C:C6     | 2.53                     | 0.43              |
| 1:AS:2184:G:H21    | 1:AS:2186:A:H61    | 1.67                     | 0.43              |
| 1:AS:3013:U:H2'    | 1:AS:3014:U:C6     | 2.54                     | 0.43              |
| 1:AS:3023:U:H2'    | 1:AS:3024:G:H8     | 1.84                     | 0.43              |
| 8:BA:71:ASN:HB3    | 8:BA:73:VAL:HG23   | 2.00                     | 0.43              |
| 10:BC:239:MET:HB2  | 10:BC:244:ASN:HD21 | 1.84                     | 0.43              |
| 13:BF:50:ALA:HB2   | 13:BF:65:ILE:HG13  | 2.01                     | 0.43              |
| 14:BG:122:LYS:HE2  | 36:CC:119:LYS:HZ3  | 1.84                     | 0.43              |
| 26:BS:139:ILE:HG22 | 36:CC:33:VAL:HG21  | 2.01                     | 0.43              |
| 39:CF:16:ARG:HH21  | 39:CF:70:PRO:HD3   | 1.82                     | 0.43              |
| 39:CF:24:ILE:HA    | 39:CF:76:THR:O     | 2.18                     | 0.43              |
| 46:CM:188:U:H1'    | 46:CM:194:G:N2     | 2.34                     | 0.43              |
| 46:CM:203:U:C2     | 46:CM:204:A:C8     | 3.07                     | 0.43              |
| 46:CM:269:A:C2     | 46:CM:283:G:C6     | 3.07                     | 0.43              |
| 46:CM:413:C:O2'    | 46:CM:416:G:O6     | 2.32                     | 0.43              |
| 46:CM:496:G:H2'    | 46:CM:497:U:O4'    | 2.19                     | 0.43              |
| 46:CM:945:U:H5'    | 60:DA:55:ARG:HD3   | 2.00                     | 0.43              |
| 46:CM:1158:C:H2'   | 46:CM:1159:C:H6    | 1.84                     | 0.43              |
| 46:CM:1537:A:H2'   | 46:CM:1538:U:H6    | 1.83                     | 0.43              |
| 46:CM:1745:U:O4    | 86:CM:1822:GET:N12 | 2.51                     | 0.43              |
| 46:CM:1766:U:H2'   | 46:CM:1768:A:OP2   | 2.19                     | 0.43              |
| 48:CO:175:GLU:HA   | 48:CO:187:LYS:HZ2  | 1.84                     | 0.43              |
| 52:CS:91:GLU:HA    | 52:CS:94:THR:HG22  | 2.01                     | 0.43              |
| 54:CU:126:VAL:O    | 54:CU:126:VAL:HG23 | 2.17                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:CU:128:PRO:O   | 54:CU:129:THR:C  | 2.61                     | 0.43              |
| 57:CX:52:LYS:HE2  | 57:CX:54:TYR:HE2 | 1.84                     | 0.43              |
| 62:DC:58:LYS:HE2  | 62:DC:58:LYS:HB3 | 1.81                     | 0.43              |
| 65:DF:138:THR:O   | 65:DF:142:SER:OG | 2.36                     | 0.43              |
| 79:DT:40:LYS:CE   | 79:DT:67:HIS:HA  | 2.49                     | 0.43              |
| 81:P0:43:LYS:C    | 81:P0:45:LEU:H   | 2.26                     | 0.43              |
| 1:1:268:A:C4      | 16:v:12:ARG:HG2  | 2.54                     | 0.42              |
| 1:1:512:A:C6      | 1:1:573:G:C6     | 3.06                     | 0.42              |
| 1:1:962:U:H2'     | 1:1:963:A:C8     | 2.54                     | 0.42              |
| 1:1:982:U:O2'     | 9:o:120:ALA:O    | 2.37                     | 0.42              |
| 1:1:1779:U:H2'    | 1:1:1780:A:C8    | 2.53                     | 0.42              |
| 1:1:2328:C:O3'    | 18:x:68:GLY:HA3  | 2.19                     | 0.42              |
| 1:1:2719:A:H5'    | 7:m:175:HIS:HA   | 2.00                     | 0.42              |
| 1:1:2852:U:H1'    | 5:k:250:ALA:HB3  | 2.00                     | 0.42              |
| 1:1:2899:C:H2'    | 1:1:2900:C:H6    | 1.82                     | 0.42              |
| 1:1:3133:G:C6     | 1:1:3253:G:C6    | 3.07                     | 0.42              |
| 1:1:3135:A:H2'    | 1:1:3136:C:H6    | 1.84                     | 0.42              |
| 2:3:43:U:H4'      | 13:s:140:ARG:O   | 2.18                     | 0.42              |
| 7:m:40:HIS:CE1    | 22:2:69:LYS:HA   | 2.54                     | 0.42              |
| 23:5:55:SER:O     | 23:5:66:VAL:HA   | 2.18                     | 0.42              |
| 25:7:124:LYS:HA   | 25:7:127:LYS:HD3 | 2.00                     | 0.42              |
| 45:i:128:GLU:O    | 45:i:132:GLU:HG3 | 2.18                     | 0.42              |
| 46:B:182:C:H2'    | 46:B:183:C:H6    | 1.84                     | 0.42              |
| 46:B:217:A:C5     | 46:B:218:A:C8    | 3.07                     | 0.42              |
| 46:B:604:A:H4'    | 46:B:605:G:H3'   | 2.01                     | 0.42              |
| 46:B:1123:A:H2'   | 46:B:1124:A:H8   | 1.83                     | 0.42              |
| 46:B:1198:G:N2    | 46:B:1436:U:O2   | 2.32                     | 0.42              |
| 46:B:1318:C:H2'   | 46:B:1319:U:H6   | 1.83                     | 0.42              |
| 46:B:1730:U:H2'   | 46:B:1731:A:H8   | 1.84                     | 0.42              |
| 51:G:185:GLY:HA3  | 51:G:224:ASN:OD1 | 2.19                     | 0.42              |
| 56:L:29:LYS:HA    | 77:g:40:TYR:CE1  | 2.54                     | 0.42              |
| 63:S:40:PRO:O     | 63:S:43:LEU:N    | 2.49                     | 0.42              |
| 65:U:67:GLU:HA    | 65:U:70:VAL:HG22 | 2.01                     | 0.42              |
| 68:X:71:ARG:HB2   | 68:X:83:TRP:CE2  | 2.53                     | 0.42              |
| 73:c:9:GLY:O      | 73:c:34:LYS:HG3  | 2.19                     | 0.42              |
| 76:f:39:CYS:HB2   | 76:f:42:CYS:H    | 1.83                     | 0.42              |
| 79:AR:25:THR:HG21 | 79:AR:291:TRP:O  | 2.19                     | 0.42              |
| 1:AS:60:A:C4      | 1:AS:61:A:C8     | 3.06                     | 0.42              |
| 1:AS:117:U:C5     | 1:AS:122:A:N6    | 2.87                     | 0.42              |
| 1:AS:1330:U:H2'   | 1:AS:1331:U:C6   | 2.54                     | 0.42              |
| 1:AS:2330:A:H2'   | 1:AS:2331:G:H8   | 1.84                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AS:2367:C:H2'    | 1:AS:2368:A:H8    | 1.84                     | 0.42              |
| 1:AS:2659:G:H4'    | 7:AZ:7:PHE:CE2    | 2.54                     | 0.42              |
| 1:AS:2732:C:N3     | 43:CJ:63:LYS:HE3  | 2.33                     | 0.42              |
| 1:AS:2773:A:H2'    | 1:AS:2774:A:H2'   | 2.01                     | 0.42              |
| 1:AS:3068:C:H2'    | 1:AS:3069:U:C6    | 2.54                     | 0.42              |
| 4:AW:5:ILE:HG12    | 4:AW:8:GLN:HG3    | 2.01                     | 0.42              |
| 6:AY:61:THR:HG22   | 6:AY:63:ALA:N     | 2.33                     | 0.42              |
| 8:BA:145:LEU:HD23  | 8:BA:145:LEU:HA   | 1.77                     | 0.42              |
| 10:BC:34:ASN:HD22  | 10:BC:39:GLN:HE21 | 1.62                     | 0.42              |
| 13:BF:49:LYS:HB3   | 13:BF:62:ASN:HA   | 2.00                     | 0.42              |
| 14:BG:144:SER:OG   | 14:BG:145:ALA:N   | 2.51                     | 0.42              |
| 17:BJ:109:VAL:HB   | 17:BJ:161:ARG:CD  | 2.49                     | 0.42              |
| 28:BU:17:ARG:HA    | 35:CB:73:GLN:O    | 2.19                     | 0.42              |
| 36:CC:80:LEU:O     | 36:CC:81:ARG:C    | 2.62                     | 0.42              |
| 46:CM:504:A:N6     | 77:DR:27:PRO:HB3  | 2.34                     | 0.42              |
| 46:CM:598:U:OP2    | 70:DK:108:GLY:HA2 | 2.19                     | 0.42              |
| 46:CM:610:U:OP2    | 70:DK:5:LYS:NZ    | 2.47                     | 0.42              |
| 46:CM:631:U:H5''   | 70:DK:8:GLY:HA3   | 2.00                     | 0.42              |
| 46:CM:728:U:P      | 54:CU:103:ARG:HA  | 2.60                     | 0.42              |
| 46:CM:1149:G:H2'   | 46:CM:1150:G:H8   | 1.84                     | 0.42              |
| 46:CM:1289:G:OP2   | 46:CM:1290:U:O2'  | 2.30                     | 0.42              |
| 46:CM:1482:C:O2'   | 46:CM:1506:U:O2   | 2.33                     | 0.42              |
| 46:CM:1508:G:O2'   | 46:CM:1510:G:OP2  | 2.31                     | 0.42              |
| 46:CM:1515:U:H2'   | 46:CM:1516:C:C6   | 2.54                     | 0.42              |
| 47:CN:123:VAL:HG13 | 47:CN:129:ASP:HB2 | 2.00                     | 0.42              |
| 48:CO:88:VAL:O     | 48:CO:88:VAL:HG13 | 2.19                     | 0.42              |
| 48:CO:133:TYR:CZ   | 48:CO:220:GLN:OE1 | 2.71                     | 0.42              |
| 51:CR:32:SER:OG    | 51:CR:81:THR:HG23 | 2.19                     | 0.42              |
| 51:CR:141:THR:OG1  | 51:CR:145:ARG:HB2 | 2.19                     | 0.42              |
| 52:CS:166:ARG:HB2  | 75:DP:46:GLY:HA3  | 2.00                     | 0.42              |
| 61:DB:84:THR:O     | 61:DB:123:ARG:HD2 | 2.18                     | 0.42              |
| 62:DC:8:LYS:O      | 62:DC:9:LYS:HG2   | 2.19                     | 0.42              |
| 62:DC:111:MET:HG2  | 62:DC:119:PHE:CZ  | 2.54                     | 0.42              |
| 70:DK:107:PHE:CD2  | 70:DK:114:LYS:HB3 | 2.54                     | 0.42              |
| 73:DN:9:GLY:O      | 73:DN:34:LYS:HG3  | 2.19                     | 0.42              |
| 78:DS:160:ARG:CZ   | 78:DS:176:ASN:HB2 | 2.49                     | 0.42              |
| 1:1:246:U:OP1      | 14:BG:137:SER:HA  | 2.19                     | 0.42              |
| 1:1:523:G:C6       | 1:1:564:G:C6      | 3.07                     | 0.42              |
| 1:1:542:U:O5'      | 1:1:542:U:H6      | 2.02                     | 0.42              |
| 1:1:629:A:H2       | 34:AG:91:PRO:HG2  | 1.84                     | 0.42              |
| 1:1:1017:G:N1      | 1:1:1028:C:C4     | 2.87                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:1347:U:O2    | 1:1:1347:U:H2'    | 2.20                     | 0.42              |
| 1:1:1549:U:H4'   | 1:1:1550:U:H5'    | 2.00                     | 0.42              |
| 1:1:1944:G:H2'   | 1:1:1945:A:H8     | 1.82                     | 0.42              |
| 1:1:2256:C:H2'   | 1:1:2257:A:H5''   | 2.00                     | 0.42              |
| 1:1:3240:U:H5''  | 34:AG:68:TRP:HZ2  | 1.84                     | 0.42              |
| 1:1:3256:G:C2    | 1:1:3257:A:C5     | 3.07                     | 0.42              |
| 1:1:3335:A:H2'   | 1:1:3336:G:C8     | 2.54                     | 0.42              |
| 35:AH:16:ARG:HG2 | 35:AH:37:LYS:HD3  | 2.01                     | 0.42              |
| 45:i:135:GLU:HG2 | 45:i:136:ASN:N    | 2.33                     | 0.42              |
| 46:B:119:A:H1'   | 46:B:395:A:C4     | 2.54                     | 0.42              |
| 46:B:217:A:H5''  | 46:B:816:U:O2     | 2.18                     | 0.42              |
| 46:B:449:G:H2'   | 46:B:451:C:C5     | 2.54                     | 0.42              |
| 46:B:752:U:C5    | 56:L:143:ILE:HG12 | 2.54                     | 0.42              |
| 46:B:770:C:P     | 46:B:770:C:O4'    | 2.77                     | 0.42              |
| 46:B:1191:U:OP2  | 46:B:1192:C:O2'   | 2.19                     | 0.42              |
| 46:B:1704:C:C2   | 46:B:1705:G:C8    | 3.08                     | 0.42              |
| 46:B:1772:U:H2'  | 46:B:1773:G:H8    | 1.84                     | 0.42              |
| 50:F:104:GLU:HG2 | 50:F:174:ARG:HD3  | 2.01                     | 0.42              |
| 51:G:45:VAL:HA   | 51:G:61:VAL:HG21  | 2.01                     | 0.42              |
| 52:H:58:LEU:HD12 | 52:H:138:VAL:HG12 | 2.01                     | 0.42              |
| 59:O:105:GLN:H   | 59:O:105:GLN:HG2  | 1.53                     | 0.42              |
| 67:W:47:TYR:O    | 67:W:49:ILE:N     | 2.48                     | 0.42              |
| 76:f:24:CYS:HB2  | 76:f:42:CYS:SG    | 2.50                     | 0.42              |
| 1:AS:40:G:N2     | 1:AS:2775:A:N7    | 2.67                     | 0.42              |
| 1:AS:129:G:C6    | 1:AS:138:G:C6     | 3.07                     | 0.42              |
| 1:AS:352:A:N1    | 1:AS:365:A:H5''   | 2.34                     | 0.42              |
| 1:AS:414:U:H2'   | 1:AS:415:G:H8     | 1.84                     | 0.42              |
| 1:AS:798:C:H2'   | 1:AS:799:C:C6     | 2.55                     | 0.42              |
| 1:AS:1079:G:H2'  | 1:AS:1080:A:C8    | 2.53                     | 0.42              |
| 1:AS:1379:G:OP1  | 6:AY:204:ARG:HD3  | 2.19                     | 0.42              |
| 1:AS:1486:A:O2'  | 38:CE:12:HIS:O    | 2.26                     | 0.42              |
| 1:AS:1762:G:H2'  | 1:AS:1763:C:C6    | 2.54                     | 0.42              |
| 1:AS:2183:U:HO2' | 1:AS:2184:G:P     | 2.42                     | 0.42              |
| 1:AS:2243:C:H2'  | 1:AS:2244:U:C6    | 2.54                     | 0.42              |
| 1:AS:2384:C:H2'  | 1:AS:2385:C:H6    | 1.84                     | 0.42              |
| 1:AS:2515:G:H1'  | 1:AS:2516:U:O5'   | 2.18                     | 0.42              |
| 1:AS:2873:G:N2   | 1:AS:3002:G:O2'   | 2.52                     | 0.42              |
| 3:AU:113:U:H5''  | 40:CG:7:PHE:CB    | 2.49                     | 0.42              |
| 10:BC:46:ASN:CB  | 26:BS:26:VAL:HG13 | 2.49                     | 0.42              |
| 80:BE:4:ARG:CZ   | 80:BE:99:ILE:HG13 | 2.49                     | 0.42              |
| 18:BK:4:TYR:CZ   | 18:BK:18:ARG:HG3  | 2.53                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:BY:22:VAL:HG21  | 32:BY:30:LYS:HD3  | 2.01                     | 0.42              |
| 36:CC:35:LYS:HG3   | 36:CC:35:LYS:O    | 2.18                     | 0.42              |
| 39:CF:20:ILE:HG23  | 39:CF:45:VAL:HG13 | 2.00                     | 0.42              |
| 45:CL:112:LYS:HD2  | 45:CL:116:GLU:HG3 | 2.01                     | 0.42              |
| 46:CM:1:U:C2       | 46:CM:3:U:C4      | 3.07                     | 0.42              |
| 46:CM:71:A:C6      | 46:CM:81:G:C6     | 3.07                     | 0.42              |
| 46:CM:75:U:H2'     | 46:CM:76:A:C2     | 2.54                     | 0.42              |
| 46:CM:94:U:O2'     | 51:CR:7:LYS:HB2   | 2.19                     | 0.42              |
| 46:CM:98:U:H2'     | 46:CM:99:C:C6     | 2.55                     | 0.42              |
| 46:CM:479:A:H2'    | 46:CM:480:U:H6    | 1.85                     | 0.42              |
| 46:CM:680:C:O2'    | 46:CM:681:C:H6    | 2.02                     | 0.42              |
| 46:CM:883:A:N3     | 46:CM:884:G:H1'   | 2.32                     | 0.42              |
| 47:CN:200:ASP:O    | 47:CN:203:PHE:HB2 | 2.18                     | 0.42              |
| 48:CO:69:CYS:O     | 48:CO:72:ASP:OD1  | 2.36                     | 0.42              |
| 53:CT:32:MET:HE2   | 53:CT:100:CYS:HB2 | 2.01                     | 0.42              |
| 53:CT:57:ASP:OD2   | 53:CT:72:ARG:NH1  | 2.47                     | 0.42              |
| 65:DF:49:LYS:NZ    | 65:DF:80:LYS:HB3  | 2.35                     | 0.42              |
| 65:DF:87:ASN:HB2   | 65:DF:99:HIS:CE1  | 2.53                     | 0.42              |
| 78:DS:181:GLN:HE22 | 78:DS:189:THR:C   | 2.27                     | 0.42              |
| 1:1:1018:U:H2'     | 1:1:1019:U:C5     | 2.53                     | 0.42              |
| 1:1:1093:G:H4'     | 22:2:129:LYS:HG2  | 2.00                     | 0.42              |
| 1:1:1598:A:H4'     | 20:z:10:LEU:HD11  | 2.01                     | 0.42              |
| 1:1:1865:C:H4'     | 1:1:3049:A:O2'    | 2.20                     | 0.42              |
| 1:1:2381:G:C8      | 1:1:2842:C:H4'    | 2.54                     | 0.42              |
| 1:1:2511:G:C2      | 1:1:2525:A:C2     | 3.07                     | 0.42              |
| 1:1:3191:A:C4      | 1:1:3192:A:C8     | 3.07                     | 0.42              |
| 1:1:3203:A:C2      | 1:1:3215:U:H1'    | 2.55                     | 0.42              |
| 4:j:129:THR:OG1    | 4:j:132:ASN:ND2   | 2.38                     | 0.42              |
| 10:p:95:LEU:HB3    | 10:p:133:VAL:HG21 | 2.01                     | 0.42              |
| 15:u:39:LEU:HD22   | 21:0:72:VAL:HG23  | 2.01                     | 0.42              |
| 43:AP:38:GLN:HA    | 43:AP:41:ARG:HG3  | 2.01                     | 0.42              |
| 46:B:526:U:H2'     | 46:B:527:A:O4'    | 2.19                     | 0.42              |
| 46:B:676:G:N3      | 46:B:676:G:H2'    | 2.34                     | 0.42              |
| 46:B:885:A:H2'     | 46:B:886:G:C8     | 2.54                     | 0.42              |
| 46:B:1200:C:H2'    | 46:B:1201:C:C6    | 2.54                     | 0.42              |
| 46:B:1243:U:C6     | 46:B:1244:U:H5    | 2.36                     | 0.42              |
| 46:B:1634:U:H2'    | 46:B:1635:A:H8    | 1.83                     | 0.42              |
| 46:B:1655:G:C6     | 46:B:1656:U:C4    | 3.07                     | 0.42              |
| 46:B:1655:G:H2'    | 46:B:1656:U:C6    | 2.54                     | 0.42              |
| 49:E:138:TYR:CG    | 49:E:142:ASN:HA   | 2.54                     | 0.42              |
| 63:S:88:LEU:HG     | 63:S:104:LEU:HD13 | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:S:89:VAL:HG13   | 63:S:101:LYS:HG2   | 2.01                     | 0.42              |
| 70:Z:70:LYS:HD3    | 77:g:8:LEU:HD22    | 2.02                     | 0.42              |
| 1:AS:48:A:C4       | 1:AS:279:U:H4'     | 2.54                     | 0.42              |
| 1:AS:594:C:H2'     | 1:AS:595:G:O4'     | 2.20                     | 0.42              |
| 1:AS:1141:G:OP1    | 33:BZ:45:ARG:HD2   | 2.20                     | 0.42              |
| 1:AS:1630:G:C6     | 1:AS:1636:G:C6     | 3.07                     | 0.42              |
| 1:AS:1644:A:H2'    | 1:AS:1645:U:O4'    | 2.19                     | 0.42              |
| 1:AS:2532:A:N6     | 44:CK:62:LYS:HG2   | 2.34                     | 0.42              |
| 1:AS:2534:C:H5'    | 28:BU:136:PHE:O    | 2.19                     | 0.42              |
| 1:AS:2542:C:C2     | 1:AS:2549:G:C2     | 3.07                     | 0.42              |
| 1:AS:2557:G:O6     | 10:BC:48:SER:OG    | 2.35                     | 0.42              |
| 1:AS:3199:G:H2'    | 1:AS:3200:C:C6     | 2.54                     | 0.42              |
| 4:AW:83:TYR:CZ     | 4:AW:86:GLN:HB2    | 2.53                     | 0.42              |
| 10:BC:71:LYS:HG2   | 10:BC:234:TRP:HE3  | 1.81                     | 0.42              |
| 80:BE:56:GLU:HB3   | 80:BE:58:GLU:HG3   | 1.99                     | 0.42              |
| 25:BR:108:LYS:HD3  | 25:BR:108:LYS:C    | 2.45                     | 0.42              |
| 27:BT:116:LYS:NZ   | 27:BT:127:GLU:HG2  | 2.33                     | 0.42              |
| 36:CC:109:ILE:O    | 36:CC:112:PRO:HD3  | 2.18                     | 0.42              |
| 46:CM:282:G:O6     | 53:CT:188:ARG:NH2  | 2.52                     | 0.42              |
| 46:CM:590:A:OP1    | 56:CW:39:LYS:HG3   | 2.19                     | 0.42              |
| 46:CM:740:A:H2'    | 46:CM:741:A:C8     | 2.55                     | 0.42              |
| 46:CM:740:A:HO2'   | 46:CM:741:A:P      | 2.42                     | 0.42              |
| 46:CM:814:A:H4'    | 46:CM:815:U:H5'    | 2.01                     | 0.42              |
| 46:CM:985:C:H6     | 46:CM:988:A:H8     | 1.67                     | 0.42              |
| 46:CM:1488:C:OP2   | 66:DG:102:ARG:NE   | 2.52                     | 0.42              |
| 46:CM:1644:U:O5'   | 46:CM:1645:G:H5''  | 2.18                     | 0.42              |
| 46:CM:1671:G:C6    | 46:CM:1705:G:C6    | 3.07                     | 0.42              |
| 46:CM:1783:C:O2    | 73:DN:92:ARG:HB3   | 2.19                     | 0.42              |
| 48:CO:24:PHE:CA    | 48:CO:27:LYS:HG2   | 2.48                     | 0.42              |
| 48:CO:193:ILE:O    | 48:CO:197:ILE:HG12 | 2.19                     | 0.42              |
| 54:CU:18:ALA:O     | 54:CU:21:PHE:HB2   | 2.18                     | 0.42              |
| 58:CY:66:ILE:HD13  | 58:CY:128:CYS:HB3  | 2.00                     | 0.42              |
| 62:DC:53:PRO:HA    | 62:DC:83:MET:HE1   | 2.02                     | 0.42              |
| 63:DD:10:GLY:HA3   | 63:DD:82:GLN:HB2   | 2.02                     | 0.42              |
| 65:DF:49:LYS:HA    | 65:DF:49:LYS:HD3   | 1.68                     | 0.42              |
| 70:DK:57:ILE:HD11  | 77:DR:4:VAL:HB     | 2.01                     | 0.42              |
| 78:DS:128:THR:O    | 78:DS:129:THR:OG1  | 2.35                     | 0.42              |
| 79:DT:19:TRP:HB3   | 79:DT:287:ILE:CD1  | 2.49                     | 0.42              |
| 79:DT:178:TRP:O    | 79:DT:184:SER:O    | 2.37                     | 0.42              |
| 79:DT:231:LEU:HD12 | 79:DT:232:GLU:N    | 2.33                     | 0.42              |
| 79:DT:246:ARG:O    | 79:DT:248:TRP:CD1  | 2.73                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:P0:59:VAL:HG21 | 81:P0:86:PHE:CZ    | 2.54                     | 0.42              |
| 81:P0:75:LYS:O    | 81:P0:78:PRO:HD2   | 2.19                     | 0.42              |
| 81:P0:76:LEU:HA   | 81:P0:79:PHE:CE1   | 2.52                     | 0.42              |
| 1:1:195:G:N2      | 1:1:197:A:H3'      | 2.34                     | 0.42              |
| 1:1:449:U:H2'     | 1:1:450:G:C8       | 2.55                     | 0.42              |
| 1:1:780:A:H2'     | 1:1:780:A:N3       | 2.34                     | 0.42              |
| 1:1:1029:U:O2'    | 1:1:1030:U:OP1     | 2.26                     | 0.42              |
| 1:1:1036:A:H1'    | 12:r:198:LYS:NZ    | 2.35                     | 0.42              |
| 1:1:1313:A:O2'    | 1:1:1314:A:H3'     | 2.19                     | 0.42              |
| 1:1:1428:C:O2'    | 1:1:1430:G:OP2     | 2.35                     | 0.42              |
| 1:1:1620:G:O2'    | 1:1:1639:A:N1      | 2.50                     | 0.42              |
| 1:1:2802:G:H1'    | 1:1:2833:U:C2      | 2.54                     | 0.42              |
| 1:1:2814:U:OP1    | 1:1:2816:C:N4      | 2.50                     | 0.42              |
| 1:1:2938:G:H2'    | 1:1:2939:A:C8      | 2.54                     | 0.42              |
| 2:3:60:G:H2'      | 2:3:61:C:C6        | 2.54                     | 0.42              |
| 3:4:10:A:H2'      | 3:4:11:C:C6        | 2.55                     | 0.42              |
| 5:k:182:GLN:HE21  | 5:k:184:ASN:HD21   | 1.66                     | 0.42              |
| 30:AC:58:ARG:HG2  | 30:AC:59:ALA:N     | 2.29                     | 0.42              |
| 46:B:117:U:H2'    | 46:B:118:U:O4'     | 2.19                     | 0.42              |
| 46:B:215:A:H3'    | 46:B:215:A:OP1     | 2.19                     | 0.42              |
| 46:B:260:U:O2'    | 46:B:261:C:H5'     | 2.19                     | 0.42              |
| 46:B:528:C:C4     | 46:B:529:C:C5      | 3.08                     | 0.42              |
| 46:B:787:A:C4     | 54:J:100:ARG:HD2   | 2.54                     | 0.42              |
| 46:B:985:C:H6     | 46:B:988:A:H8      | 1.68                     | 0.42              |
| 46:B:1029:U:H2'   | 46:B:1030:C:C6     | 2.54                     | 0.42              |
| 46:B:1184:G:O6    | 67:W:66:THR:HG22   | 2.18                     | 0.42              |
| 49:E:108:LEU:CD1  | 49:E:206:LEU:HB3   | 2.50                     | 0.42              |
| 51:G:31:PRO:HD2   | 51:G:38:LEU:HD11   | 2.01                     | 0.42              |
| 59:O:26:ASP:HA    | 59:O:29:LYS:CG     | 2.50                     | 0.42              |
| 62:R:72:ARG:HH21  | 62:R:93:VAL:HG11   | 1.84                     | 0.42              |
| 64:T:89:SER:C     | 64:T:91:LEU:N      | 2.75                     | 0.42              |
| 66:V:106:GLN:O    | 66:V:110:LYS:HG2   | 2.18                     | 0.42              |
| 79:AR:75:SER:HA   | 79:AR:116:ILE:HD11 | 2.01                     | 0.42              |
| 79:AR:110:ASP:OD2 | 79:AR:128:ARG:NH1  | 2.45                     | 0.42              |
| 79:AR:156:ARG:HD3 | 79:AR:156:ARG:HA   | 1.81                     | 0.42              |
| 1:AS:143:A:H2'    | 1:AS:144:G:O4'     | 2.19                     | 0.42              |
| 1:AS:194:U:H2'    | 1:AS:195:G:O4'     | 2.19                     | 0.42              |
| 1:AS:381:U:H2'    | 1:AS:382:U:C6      | 2.54                     | 0.42              |
| 1:AS:560:C:H2'    | 1:AS:561:U:H6      | 1.84                     | 0.42              |
| 1:AS:1018:U:C2'   | 1:AS:1019:U:H5''   | 2.49                     | 0.42              |
| 1:AS:1080:A:H2'   | 1:AS:1081:A:C8     | 2.55                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:1746:A:OP2    | 39:CF:28:ASN:ND2   | 2.47                     | 0.42              |
| 1:AS:1753:G:C6     | 1:AS:1765:G:C6     | 3.07                     | 0.42              |
| 1:AS:2646:A:C2     | 13:BF:124:GLY:HA3  | 2.55                     | 0.42              |
| 1:AS:3240:U:N3     | 1:AS:3242:U:O4'    | 2.48                     | 0.42              |
| 1:AS:3264:C:H2'    | 1:AS:3265:U:H6     | 1.84                     | 0.42              |
| 3:AU:5:U:OP1       | 18:BK:62:ARG:HG3   | 2.19                     | 0.42              |
| 3:AU:44:A:C2       | 3:AU:101:U:C2      | 3.06                     | 0.42              |
| 4:AW:178:PRO:O     | 4:AW:180:LEU:HD12  | 2.18                     | 0.42              |
| 6:AY:299:VAL:HG11  | 19:BL:132:PRO:HB2  | 2.00                     | 0.42              |
| 10:BC:139:HIS:NE2  | 10:BC:143:LEU:HD11 | 2.34                     | 0.42              |
| 13:BF:47:GLN:HE22  | 45:CL:32:LYS:NZ    | 2.18                     | 0.42              |
| 14:BG:76:THR:HG21  | 14:BG:103:ASN:OD1  | 2.19                     | 0.42              |
| 27:BT:63:LYS:HD3   | 27:BT:63:LYS:HA    | 1.87                     | 0.42              |
| 28:BU:75:VAL:HB    | 28:BU:80:LEU:HD11  | 2.01                     | 0.42              |
| 32:BY:18:ARG:HD3   | 32:BY:34:GLU:HB3   | 2.00                     | 0.42              |
| 39:CF:11:PHE:CZ    | 39:CF:45:VAL:HG23  | 2.55                     | 0.42              |
| 46:CM:214:U:O2'    | 46:CM:215:A:OP1    | 2.34                     | 0.42              |
| 46:CM:499:U:C4     | 46:CM:500:U:C4     | 3.07                     | 0.42              |
| 46:CM:588:C:H2'    | 46:CM:589:A:C8     | 2.55                     | 0.42              |
| 46:CM:631:U:C5'    | 70:DK:8:GLY:HA3    | 2.49                     | 0.42              |
| 46:CM:702:G:N3     | 46:CM:703:U:H1'    | 2.34                     | 0.42              |
| 46:CM:1012:A:OP1   | 46:CM:1776:G:O2'   | 2.33                     | 0.42              |
| 46:CM:1399:U:O2'   | 46:CM:1402:G:OP1   | 2.37                     | 0.42              |
| 46:CM:1470:G:H2'   | 46:CM:1471:C:H6    | 1.85                     | 0.42              |
| 46:CM:1635:A:H2'   | 46:CM:1636:C:H6    | 1.82                     | 0.42              |
| 49:CP:203:GLU:O    | 49:CP:207:LYS:HG3  | 2.20                     | 0.42              |
| 53:CT:48:TYR:OH    | 53:CT:119:ASN:O    | 2.28                     | 0.42              |
| 53:CT:120:GLU:OE1  | 53:CT:126:ASP:HB3  | 2.19                     | 0.42              |
| 54:CU:92:ARG:NH1   | 54:CU:124:ASP:OD2  | 2.41                     | 0.42              |
| 56:CW:148:VAL:HG11 | 56:CW:156:ILE:HD11 | 2.01                     | 0.42              |
| 59:CZ:68:GLU:C     | 59:CZ:70:SER:N     | 2.77                     | 0.42              |
| 59:CZ:89:ILE:HG13  | 59:CZ:90:LYS:H     | 1.84                     | 0.42              |
| 62:DC:34:THR:HG22  | 62:DC:45:PHE:CZ    | 2.55                     | 0.42              |
| 68:DI:38:LYS:HD3   | 68:DI:49:GLU:HG3   | 2.02                     | 0.42              |
| 73:DN:73:TYR:CD2   | 73:DN:83:ILE:HD13  | 2.54                     | 0.42              |
| 79:DT:67:HIS:CG    | 79:DT:68:ILE:H     | 2.38                     | 0.42              |
| 79:DT:126:ALA:HB1  | 79:DT:152:VAL:HG12 | 2.00                     | 0.42              |
| 79:DT:250:ALA:HA   | 79:DT:260:PHE:CD2  | 2.55                     | 0.42              |
| 81:P0:73:PHE:CD2   | 81:P0:76:LEU:HB2   | 2.55                     | 0.42              |
| 82:12:148:PRO:HA   | 82:12:151:ILE:HG12 | 2.00                     | 0.42              |
| 1:1:117:U:C5       | 1:1:122:A:N6       | 2.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:392:G:H22     | 1:1:400:G:H1      | 1.67                     | 0.42              |
| 1:1:898:G:H2'     | 1:1:899:U:O4'     | 2.19                     | 0.42              |
| 1:1:1273:C:H2'    | 1:1:1274:A:H8     | 1.82                     | 0.42              |
| 1:1:1379:G:OP1    | 6:l:204:ARG:HD3   | 2.19                     | 0.42              |
| 1:1:1386:A:H5'    | 1:1:1386:A:N3     | 2.34                     | 0.42              |
| 1:1:1460:G:N2     | 1:1:1462:G:H3'    | 2.34                     | 0.42              |
| 1:1:1586:G:C2     | 1:1:1587:G:C8     | 3.07                     | 0.42              |
| 1:1:2146:A:C6     | 1:1:2148:U:H1'    | 2.55                     | 0.42              |
| 1:1:2493:A:H5''   | 16:v:28:TRP:CD1   | 2.54                     | 0.42              |
| 1:1:2933:G:H2'    | 1:1:2934:U:H6     | 1.83                     | 0.42              |
| 1:1:3038:U:C2     | 1:1:3039:C:C5     | 3.08                     | 0.42              |
| 2:3:13:A:H2       | 7:m:21:ARG:HB2    | 1.84                     | 0.42              |
| 5:k:160:VAL:HG12  | 5:k:181:ILE:O     | 2.19                     | 0.42              |
| 6:l:111:ASN:HB2   | 16:v:201:ARG:O    | 2.18                     | 0.42              |
| 12:r:4:ARG:NH1    | 12:r:99:ILE:HG13  | 2.35                     | 0.42              |
| 13:s:37:LEU:HD23  | 13:s:37:LEU:HA    | 1.88                     | 0.42              |
| 18:x:166:ILE:HG22 | 18:x:168:LEU:HD21 | 2.00                     | 0.42              |
| 21:0:41:TYR:O     | 21:0:45:LEU:HD23  | 2.20                     | 0.42              |
| 31:AD:86:LEU:HD23 | 31:AD:86:LEU:HA   | 1.90                     | 0.42              |
| 36:AI:70:TYR:HB3  | 36:AI:76:ILE:HG22 | 2.01                     | 0.42              |
| 46:B:67:A:N6      | 46:B:83:G:O2'     | 2.52                     | 0.42              |
| 46:B:451:C:O2     | 46:B:451:C:H2'    | 2.20                     | 0.42              |
| 46:B:583:A:H2'    | 46:B:584:G:H8     | 1.84                     | 0.42              |
| 46:B:1325:U:O4'   | 46:B:1364:U:H5''  | 2.20                     | 0.42              |
| 46:B:1377:A:H2'   | 46:B:1378:U:C6    | 2.54                     | 0.42              |
| 50:F:158:MET:HE2  | 50:F:158:MET:HB2  | 1.83                     | 0.42              |
| 54:J:7:SER:HB3    | 54:J:40:LYS:O     | 2.20                     | 0.42              |
| 70:Z:62:LYS:H     | 70:Z:116:ASP:HB2  | 1.84                     | 0.42              |
| 71:a:27:VAL:O     | 71:a:68:LYS:HA    | 2.19                     | 0.42              |
| 72:b:69:LEU:HD23  | 72:b:69:LEU:HA    | 1.92                     | 0.42              |
| 1:AS:83:C:O2'     | 1:AS:100:G:O6     | 2.33                     | 0.42              |
| 1:AS:242:C:O2'    | 1:AS:243:G:H8     | 2.02                     | 0.42              |
| 1:AS:487:C:H3'    | 1:AS:488:G:H8     | 1.85                     | 0.42              |
| 1:AS:1149:A:O2'   | 1:AS:1150:A:H5'   | 2.20                     | 0.42              |
| 1:AS:2236:U:O4    | 46:CM:1633:C:H4'  | 2.20                     | 0.42              |
| 1:AS:2785:A:H2'   | 1:AS:2786:G:O4'   | 2.18                     | 0.42              |
| 1:AS:2856:C:H2'   | 1:AS:2857:C:H6    | 1.85                     | 0.42              |
| 1:AS:2995:U:H2'   | 1:AS:2996:A:H8    | 1.85                     | 0.42              |
| 1:AS:3197:G:C6    | 1:AS:3221:G:C6    | 3.07                     | 0.42              |
| 2:AT:45:A:H2'     | 2:AT:46:A:C8      | 2.54                     | 0.42              |
| 3:AU:37:A:H5''    | 3:AU:39:G:O4'     | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AU:42:G:N2       | 3:AU:103:G:H1'     | 2.34                     | 0.42              |
| 3:AU:51:G:C8       | 40:CG:27:ILE:HD11  | 2.55                     | 0.42              |
| 11:BD:13:PRO:HG2   | 11:BD:16:VAL:HG21  | 2.01                     | 0.42              |
| 13:BF:108:GLU:HB3  | 13:BF:122:ILE:HD11 | 2.01                     | 0.42              |
| 16:BI:20:ARG:NH1   | 37:CD:51:PRO:HG3   | 2.33                     | 0.42              |
| 23:BP:74:PHE:CZ    | 23:BP:79:LEU:HB2   | 2.55                     | 0.42              |
| 24:BQ:120:LYS:HB2  | 24:BQ:137:VAL:C    | 2.44                     | 0.42              |
| 26:BS:47:GLN:O     | 36:CC:77:PRO:HG3   | 2.20                     | 0.42              |
| 26:BS:82:LEU:HD21  | 26:BS:132:ALA:HB1  | 2.00                     | 0.42              |
| 28:BU:32:GLY:HA2   | 28:BU:38:PHE:O     | 2.19                     | 0.42              |
| 40:CG:41:ARG:HD2   | 40:CG:41:ARG:HA    | 1.80                     | 0.42              |
| 46:CM:724:G:C4     | 46:CM:725:A:C8     | 3.07                     | 0.42              |
| 46:CM:1016:U:H4'   | 46:CM:1017:G:OP2   | 2.19                     | 0.42              |
| 46:CM:1243:U:H4'   | 57:CX:2:LEU:HG     | 2.01                     | 0.42              |
| 46:CM:1298:A:N3    | 46:CM:1300:U:H5'   | 2.34                     | 0.42              |
| 46:CM:1566:U:H1'   | 63:DD:138:GLN:CD   | 2.44                     | 0.42              |
| 49:CP:217:TYR:HE1  | 68:DI:10:GLU:OE2   | 2.03                     | 0.42              |
| 51:CR:100:ARG:HH12 | 51:CR:118:GLU:HG2  | 1.84                     | 0.42              |
| 64:DE:78:ARG:HA    | 64:DE:78:ARG:HD3   | 1.72                     | 0.42              |
| 65:DF:36:ARG:HG2   | 65:DF:102:ALA:HA   | 2.02                     | 0.42              |
| 79:DT:65:HIS:CD2   | 79:DT:93:TRP:HZ2   | 2.38                     | 0.42              |
| 81:P0:16:ARG:HD3   | 81:P0:66:PHE:CE2   | 2.54                     | 0.42              |
| 82:12:120:SER:C    | 82:12:122:GLY:N    | 2.78                     | 0.42              |
| 1:1:35:C:H4'       | 1:1:804:A:C2       | 2.55                     | 0.42              |
| 1:1:88:G:H21       | 1:1:281:G:C4'      | 2.32                     | 0.42              |
| 1:1:96:U:H2'       | 1:1:97:G:C8        | 2.55                     | 0.42              |
| 1:1:151:U:OP2      | 36:AI:103:LYS:HB2  | 2.20                     | 0.42              |
| 1:1:180:U:H4'      | 38:AK:75:LYS:CG    | 2.50                     | 0.42              |
| 1:1:304:G:H3'      | 1:1:304:G:OP2      | 2.20                     | 0.42              |
| 1:1:406:G:H1'      | 3:4:16:G:N2        | 2.35                     | 0.42              |
| 1:1:498:C:H5''     | 8:n:25:ARG:CZ      | 2.49                     | 0.42              |
| 1:1:1237:U:O2'     | 1:1:1239:G:N7      | 2.47                     | 0.42              |
| 1:1:1440:G:H2'     | 1:1:1441:U:O4'     | 2.19                     | 0.42              |
| 1:1:2078:A:N3      | 1:1:2078:A:H3'     | 2.35                     | 0.42              |
| 1:1:2180:C:H5''    | 4:j:226:SER:N      | 2.35                     | 0.42              |
| 1:1:2618:C:H5''    | 12:r:119:TRP:CG    | 2.55                     | 0.42              |
| 1:1:2719:A:H2'     | 1:1:2720:A:C8      | 2.54                     | 0.42              |
| 1:1:2739:U:H2'     | 1:1:2740:U:H6      | 1.84                     | 0.42              |
| 1:1:2781:C:H5''    | 1:1:2928:A:H4'     | 2.02                     | 0.42              |
| 1:1:3199:G:H2'     | 1:1:3200:C:H6      | 1.85                     | 0.42              |
| 2:3:31:U:H4'       | 7:m:218:LYS:HZ1    | 1.85                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:l:159:SER:HA    | 6:l:214:ASN:HB2    | 2.01                     | 0.42              |
| 8:n:39:LEU:CD1    | 8:n:53:TYR:HB2     | 2.50                     | 0.42              |
| 8:n:164:SER:OG    | 8:n:166:LYS:NZ     | 2.53                     | 0.42              |
| 17:w:74:PHE:HB3   | 17:w:79:ARG:CB     | 2.49                     | 0.42              |
| 18:x:13:LYS:HD2   | 18:x:152:GLU:OE1   | 2.20                     | 0.42              |
| 45:i:101:LYS:CB   | 46:B:573:C:H5''    | 2.50                     | 0.42              |
| 46:B:273:C:H2'    | 46:B:274:C:O4'     | 2.20                     | 0.42              |
| 46:B:822:G:H3'    | 46:B:823:G:H4'     | 2.02                     | 0.42              |
| 46:B:943:U:H2'    | 60:P:14:SER:OG     | 2.19                     | 0.42              |
| 46:B:1064:U:H2'   | 46:B:1065:U:H6     | 1.83                     | 0.42              |
| 46:B:1071:A:H2'   | 46:B:1072:A:C8     | 2.54                     | 0.42              |
| 46:B:1107:G:N2    | 46:B:1110:A:OP2    | 2.52                     | 0.42              |
| 46:B:1581:G:H2'   | 46:B:1582:U:O4'    | 2.19                     | 0.42              |
| 46:B:1741:A:C2    | 86:B:1851:GET:H411 | 2.54                     | 0.42              |
| 46:B:1756:U:H1'   | 61:Q:131:ARG:HB3   | 2.01                     | 0.42              |
| 47:C:122:VAL:HG22 | 47:C:144:ILE:HB    | 2.02                     | 0.42              |
| 48:D:167:LYS:HD3  | 48:D:170:GLU:OE2   | 2.19                     | 0.42              |
| 50:F:143:LEU:HA   | 50:F:180:GLN:NE2   | 2.33                     | 0.42              |
| 50:F:214:ASP:CG   | 50:F:215:GLU:H     | 2.15                     | 0.42              |
| 52:H:217:LEU:HD23 | 52:H:217:LEU:HA    | 1.86                     | 0.42              |
| 55:K:81:VAL:HG22  | 55:K:102:VAL:HG12  | 2.02                     | 0.42              |
| 65:U:3:LEU:HB2    | 72:b:82:GLN:CD     | 2.44                     | 0.42              |
| 1:AS:29:G:C6      | 1:AS:54:G:C6       | 3.08                     | 0.42              |
| 1:AS:699:G:H2'    | 1:AS:700:C:C6      | 2.54                     | 0.42              |
| 1:AS:1093:G:H2'   | 1:AS:1093:G:N3     | 2.35                     | 0.42              |
| 1:AS:1154:A:H2'   | 1:AS:1155:A:H4'    | 2.00                     | 0.42              |
| 1:AS:1356:U:O4'   | 6:AY:308:GLN:HB2   | 2.19                     | 0.42              |
| 1:AS:1738:U:H2'   | 1:AS:1739:G:C8     | 2.54                     | 0.42              |
| 1:AS:1762:G:HO2'  | 1:AS:1763:C:P      | 2.43                     | 0.42              |
| 1:AS:2595:G:C4    | 1:AS:2596:G:C8     | 3.08                     | 0.42              |
| 1:AS:2625:C:H1'   | 1:AS:2666:A:C2     | 2.54                     | 0.42              |
| 1:AS:3271:U:OP1   | 5:AX:269:GLN:NE2   | 2.52                     | 0.42              |
| 1:AS:3290:G:O3'   | 32:BY:102:GLY:HA2  | 2.19                     | 0.42              |
| 13:BF:92:ARG:HG2  | 13:BF:94:LYS:H     | 1.84                     | 0.42              |
| 14:BG:57:VAL:CG2  | 14:BG:149:VAL:HG13 | 2.48                     | 0.42              |
| 14:BG:78:ALA:C    | 14:BG:109:PHE:HE1  | 2.26                     | 0.42              |
| 18:BK:138:ALA:HB1 | 18:BK:140:GLN:HG3  | 2.02                     | 0.42              |
| 21:BN:10:ILE:HG12 | 21:BN:26:ARG:HG3   | 2.02                     | 0.42              |
| 26:BS:38:LEU:HD12 | 26:BS:39:LYS:H     | 1.85                     | 0.42              |
| 26:BS:73:MET:HG3  | 26:BS:142:ILE:CD1  | 2.40                     | 0.42              |
| 36:CC:5:LYS:HB2   | 36:CC:8:GLU:HG3    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:CF:78:LEU:HD23 | 39:CF:78:LEU:HA   | 1.92                     | 0.42              |
| 46:CM:231:C:H4'   | 46:CM:232:G:H5''  | 2.01                     | 0.42              |
| 46:CM:451:C:O2    | 46:CM:451:C:H2'   | 2.20                     | 0.42              |
| 46:CM:529:C:O2'   | 46:CM:530:U:OP1   | 2.34                     | 0.42              |
| 46:CM:946:U:C2    | 46:CM:947:C:C5    | 3.07                     | 0.42              |
| 46:CM:947:C:OP2   | 60:DA:70:LYS:HE2  | 2.20                     | 0.42              |
| 46:CM:1730:U:H2'  | 46:CM:1731:A:H8   | 1.85                     | 0.42              |
| 48:CO:26:ARG:O    | 48:CO:50:ARG:N    | 2.53                     | 0.42              |
| 48:CO:56:ASN:O    | 48:CO:57:ALA:C    | 2.62                     | 0.42              |
| 48:CO:68:VAL:HG22 | 48:CO:69:CYS:N    | 2.33                     | 0.42              |
| 48:CO:105:PHE:HZ  | 48:CO:211:HIS:HB3 | 1.84                     | 0.42              |
| 52:CS:124:LEU:O   | 52:CS:125:THR:OG1 | 2.29                     | 0.42              |
| 60:DA:136:PRO:HG2 | 60:DA:139:TRP:HB2 | 2.00                     | 0.42              |
| 75:DP:25:VAL:CG2  | 75:DP:43:ASN:HB3  | 2.49                     | 0.42              |
| 78:DS:156:VAL:O   | 78:DS:157:GLU:C   | 2.61                     | 0.42              |
| 79:DT:50:GLY:HA3  | 79:DT:54:GLN:C    | 2.45                     | 0.42              |
| 79:DT:75:SER:C    | 79:DT:77:ASP:H    | 2.26                     | 0.42              |
| 79:DT:294:ASP:OD1 | 79:DT:294:ASP:N   | 2.50                     | 0.42              |
| 1:1:7:C:H2'       | 1:1:8:U:C6        | 2.54                     | 0.42              |
| 1:1:103:G:O2'     | 1:1:696:U:O2      | 2.29                     | 0.42              |
| 1:1:308:A:H1'     | 1:1:2200:A:N3     | 2.35                     | 0.42              |
| 1:1:754:C:OP1     | 43:AP:15:LYS:NZ   | 2.50                     | 0.42              |
| 1:1:976:A:H3'     | 1:1:976:A:C8      | 2.54                     | 0.42              |
| 1:1:1678:U:H4'    | 1:1:1680:U:O4     | 2.20                     | 0.42              |
| 1:1:2175:C:H4'    | 1:1:2176:A:C8     | 2.54                     | 0.42              |
| 1:1:2270:U:O2'    | 46:B:1643:U:O2'   | 2.33                     | 0.42              |
| 1:1:2961:U:H2'    | 1:1:2962:G:O4'    | 2.20                     | 0.42              |
| 1:1:3035:C:H2'    | 1:1:3036:U:H6     | 1.85                     | 0.42              |
| 3:4:75:G:H2'      | 3:4:76:C:H6       | 1.84                     | 0.42              |
| 7:m:289:LYS:HA    | 7:m:292:GLU:HG2   | 2.02                     | 0.42              |
| 11:q:86:TYR:CE2   | 11:q:151:LEU:HB2  | 2.55                     | 0.42              |
| 13:s:133:ARG:NH2  | 13:s:153:LYS:O    | 2.49                     | 0.42              |
| 23:5:38:VAL:HG13  | 23:5:50:LEU:HD22  | 2.02                     | 0.42              |
| 25:7:108:LYS:HZ3  | 53:I:154:ARG:HD3  | 1.84                     | 0.42              |
| 35:AH:58:ARG:CD   | 35:AH:59:PRO:HD2  | 2.37                     | 0.42              |
| 46:B:433:C:OP1    | 70:Z:49:ALA:HA    | 2.19                     | 0.42              |
| 46:B:586:U:H2'    | 46:B:587:C:C6     | 2.54                     | 0.42              |
| 46:B:1238:U:H2'   | 46:B:1239:U:H6    | 1.85                     | 0.42              |
| 46:B:1523:G:O2'   | 46:B:1524:C:OP1   | 2.27                     | 0.42              |
| 46:B:1612:C:H2'   | 46:B:1613:U:H6    | 1.85                     | 0.42              |
| 50:F:24:GLU:OE1   | 76:f:23:HIS:CE1   | 2.72                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:G:198:ARG:NE    | 51:G:200:LYS:HE2   | 2.34                     | 0.42              |
| 52:H:109:LYS:HB2   | 52:H:109:LYS:HE2   | 1.85                     | 0.42              |
| 57:M:44:LYS:HA     | 57:M:44:LYS:HD3    | 1.91                     | 0.42              |
| 1:AS:798:C:C2      | 1:AS:799:C:C5      | 3.08                     | 0.42              |
| 1:AS:831:G:HO2'    | 1:AS:853:G:H22     | 1.54                     | 0.42              |
| 1:AS:1099:A:H62    | 1:AS:1338:G:H21    | 1.68                     | 0.42              |
| 1:AS:1683:U:O4     | 23:BP:45:GLY:N     | 2.51                     | 0.42              |
| 1:AS:1945:A:H2'    | 1:AS:1946:U:C6     | 2.55                     | 0.42              |
| 1:AS:2339:A:H2'    | 1:AS:2340:C:C6     | 2.54                     | 0.42              |
| 5:AX:137:TYR:HA    | 5:AX:141:ALA:CB    | 2.49                     | 0.42              |
| 5:AX:283:TYR:CZ    | 5:AX:325:LYS:HB2   | 2.55                     | 0.42              |
| 7:AZ:179:ARG:HD3   | 7:AZ:179:ARG:HA    | 1.81                     | 0.42              |
| 11:BD:13:PRO:HG2   | 11:BD:16:VAL:CG2   | 2.49                     | 0.42              |
| 22:BO:45:ASN:H     | 22:BO:95:HIS:HD2   | 1.67                     | 0.42              |
| 22:BO:53:PRO:HB3   | 22:BO:91:LEU:HD21  | 2.01                     | 0.42              |
| 23:BP:83:THR:O     | 23:BP:87:LEU:HD23  | 2.20                     | 0.42              |
| 25:BR:47:ARG:NH2   | 46:CM:1712:U:H5''  | 2.35                     | 0.42              |
| 33:BZ:83:LEU:HD12  | 33:BZ:112:LYS:HD3  | 2.02                     | 0.42              |
| 46:CM:228:C:C2     | 46:CM:234:G:N2     | 2.87                     | 0.42              |
| 46:CM:282:G:N7     | 53:CT:188:ARG:NH2  | 2.55                     | 0.42              |
| 46:CM:326:A:H2'    | 46:CM:327:G:O4'    | 2.19                     | 0.42              |
| 46:CM:402:G:H2'    | 46:CM:403:C:C6     | 2.55                     | 0.42              |
| 46:CM:684:C:H2'    | 46:CM:685:C:C6     | 2.55                     | 0.42              |
| 46:CM:779:U:C2     | 46:CM:780:A:C8     | 3.08                     | 0.42              |
| 46:CM:887:G:H2'    | 46:CM:888:U:C6     | 2.55                     | 0.42              |
| 46:CM:1746:C:H2'   | 46:CM:1747:G:O4'   | 2.20                     | 0.42              |
| 47:CN:84:ARG:NH1   | 47:CN:203:PHE:O    | 2.41                     | 0.42              |
| 48:CO:171:ILE:HG12 | 48:CO:174:ARG:NH2  | 2.33                     | 0.42              |
| 48:CO:224:ASP:HB3  | 48:CO:227:SER:HB2  | 2.02                     | 0.42              |
| 50:CQ:197:ARG:HA   | 50:CQ:201:ARG:HH11 | 1.85                     | 0.42              |
| 52:CS:53:VAL:HG21  | 52:CS:62:ILE:HB    | 2.01                     | 0.42              |
| 52:CS:208:SER:O    | 52:CS:212:LYS:HG3  | 2.19                     | 0.42              |
| 54:CU:46:ASP:CB    | 54:CU:52:LYS:HG2   | 2.49                     | 0.42              |
| 57:CX:15:LEU:HD21  | 57:CX:68:LEU:HD13  | 2.00                     | 0.42              |
| 66:DG:63:ARG:CZ    | 66:DG:67:LEU:HD11  | 2.49                     | 0.42              |
| 77:DR:32:GLY:C     | 77:DR:34:ALA:N     | 2.78                     | 0.42              |
| 79:DT:156:ARG:HD3  | 79:DT:156:ARG:HA   | 1.83                     | 0.42              |
| 79:DT:195:TYR:CD2  | 79:DT:213:LYS:HD2  | 2.54                     | 0.42              |
| 1:1:377:A:O2'      | 1:1:391:A:H2       | 2.03                     | 0.42              |
| 1:1:626:U:H2'      | 1:1:627:U:O4'      | 2.20                     | 0.42              |
| 1:1:756:G:H1'      | 1:1:767:A:N6       | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1019:U:H2'    | 1:1:1020:G:C4'    | 2.49                     | 0.42              |
| 1:1:1476:G:O2'    | 1:1:1867:U:O4     | 2.30                     | 0.42              |
| 1:1:1675:A:OP1    | 23:5:97:ARG:HD2   | 2.20                     | 0.42              |
| 1:1:1928:A:C2     | 1:1:2102:G:H5''   | 2.54                     | 0.42              |
| 1:1:2404:U:H3     | 1:1:2575:G:H1     | 1.66                     | 0.42              |
| 1:1:2424:U:C2     | 1:1:2425:G:C8     | 3.08                     | 0.42              |
| 1:1:3041:G:C2     | 1:1:3042:A:C8     | 3.07                     | 0.42              |
| 1:1:3182:C:O4'    | 1:1:3231:G:N2     | 2.53                     | 0.42              |
| 3:4:5:U:H2'       | 3:4:6:U:H6        | 1.83                     | 0.42              |
| 3:4:85:G:H4'      | 3:4:86:U:OP1      | 2.20                     | 0.42              |
| 5:k:312:VAL:O     | 5:k:332:LYS:HD3   | 2.19                     | 0.42              |
| 10:p:215:LEU:O    | 10:p:219:ILE:HG12 | 2.18                     | 0.42              |
| 13:s:87:LYS:O     | 13:s:88:GLU:HG3   | 2.19                     | 0.42              |
| 14:t:101:ARG:HH22 | 14:t:112:ASN:ND2  | 2.18                     | 0.42              |
| 17:w:35:VAL:HA    | 17:w:104:LYS:O    | 2.20                     | 0.42              |
| 25:7:38:SER:O     | 25:7:42:GLN:HG3   | 2.19                     | 0.42              |
| 28:AA:68:VAL:O    | 28:AA:115:LYS:HG3 | 2.19                     | 0.42              |
| 46:B:326:A:OP2    | 58:N:56:LYS:NZ    | 2.35                     | 0.42              |
| 46:B:441:C:OP2    | 71:a:105:ARG:HB2  | 2.20                     | 0.42              |
| 46:B:608:G:OP2    | 58:N:96:LYS:NZ    | 2.45                     | 0.42              |
| 46:B:646:G:H2'    | 46:B:647:C:O4'    | 2.20                     | 0.42              |
| 46:B:769:U:O2'    | 46:B:770:C:OP2    | 2.33                     | 0.42              |
| 46:B:799:G:H8     | 46:B:799:G:OP1    | 2.03                     | 0.42              |
| 46:B:1521:G:O6    | 72:b:77:ARG:NE    | 2.45                     | 0.42              |
| 46:B:1663:U:H2'   | 46:B:1664:C:C6    | 2.55                     | 0.42              |
| 46:B:1760:C:C2    | 46:B:1776:G:C2    | 3.07                     | 0.42              |
| 57:M:46:LEU:HD23  | 57:M:66:TYR:CG    | 2.55                     | 0.42              |
| 57:M:50:THR:HB    | 57:M:55:VAL:HG23  | 2.00                     | 0.42              |
| 59:O:132:GLU:CG   | 59:O:133:ARG:H    | 2.32                     | 0.42              |
| 60:P:102:LEU:HD23 | 60:P:102:LEU:HA   | 1.88                     | 0.42              |
| 62:R:79:HIS:HE1   | 62:R:97:TYR:CZ    | 2.37                     | 0.42              |
| 79:AR:75:SER:HA   | 79:AR:116:ILE:CD1 | 2.50                     | 0.42              |
| 1:AS:208:A:H4'    | 1:AS:210:A:C8     | 2.54                     | 0.42              |
| 1:AS:413:U:H2'    | 1:AS:414:U:C6     | 2.55                     | 0.42              |
| 1:AS:504:G:OP2    | 9:BB:209:ASN:ND2  | 2.53                     | 0.42              |
| 1:AS:516:U:OP1    | 6:AY:352:PRO:HD2  | 2.20                     | 0.42              |
| 1:AS:1558:G:H5'   | 1:AS:1559:C:OP2   | 2.20                     | 0.42              |
| 1:AS:2196:G:H2'   | 1:AS:2197:A:C8    | 2.54                     | 0.42              |
| 1:AS:2232:U:H2'   | 1:AS:2239:G:N2    | 2.35                     | 0.42              |
| 1:AS:2833:U:H2'   | 1:AS:2834:U:O4'   | 2.19                     | 0.42              |
| 1:AS:2974:C:O2'   | 5:AX:180:GLU:OE2  | 2.27                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AT:13:A:OP1     | 2:AT:111:U:H1'     | 2.20                     | 0.42              |
| 2:AT:13:A:H2      | 7:AZ:21:ARG:HB2    | 1.85                     | 0.42              |
| 3:AU:113:U:H5''   | 40:CG:7:PHE:HB3    | 2.01                     | 0.42              |
| 4:AW:101:ILE:HG13 | 4:AW:165:VAL:HG22  | 2.01                     | 0.42              |
| 6:AY:326:LEU:O    | 9:BB:39:ARG:NH2    | 2.53                     | 0.42              |
| 10:BC:29:GLU:HG2  | 10:BC:31:THR:HG23  | 2.02                     | 0.42              |
| 10:BC:83:LEU:HD23 | 10:BC:83:LEU:HA    | 1.58                     | 0.42              |
| 10:BC:116:ALA:CB  | 10:BC:126:VAL:HG21 | 2.50                     | 0.42              |
| 13:BF:4:LYS:HG3   | 13:BF:6:GLN:H      | 1.84                     | 0.42              |
| 14:BG:166:GLN:O   | 14:BG:167:THR:C    | 2.62                     | 0.42              |
| 14:BG:190:LYS:O   | 14:BG:194:GLU:HG3  | 2.20                     | 0.42              |
| 21:BN:41:TYR:O    | 21:BN:45:LEU:HD23  | 2.19                     | 0.42              |
| 22:BO:102:ARG:NE  | 22:BO:102:ARG:HA   | 2.33                     | 0.42              |
| 35:CB:106:LYS:O   | 35:CB:110:ASP:HB2  | 2.20                     | 0.42              |
| 36:CC:41:LEU:HD23 | 36:CC:44:ILE:HD11  | 2.01                     | 0.42              |
| 37:CD:39:VAL:O    | 37:CD:43:VAL:HG23  | 2.20                     | 0.42              |
| 45:CL:54:LYS:O    | 45:CL:55:LYS:C     | 2.62                     | 0.42              |
| 46:CM:349:C:OP1   | 46:CM:628:A:O2'    | 2.34                     | 0.42              |
| 46:CM:497:U:H2'   | 46:CM:498:C:C6     | 2.54                     | 0.42              |
| 46:CM:988:A:H2'   | 46:CM:990:A:N7     | 2.35                     | 0.42              |
| 46:CM:1161:G:C6   | 46:CM:1450:G:C6    | 3.08                     | 0.42              |
| 46:CM:1354:U:C2'  | 46:CM:1355:A:H5'   | 2.50                     | 0.42              |
| 46:CM:1535:G:OP1  | 62:DC:18:LYS:NZ    | 2.50                     | 0.42              |
| 51:CR:95:THR:HG22 | 71:DL:16:PRO:HG2   | 2.02                     | 0.42              |
| 52:CS:26:ALA:HB3  | 63:DD:26:GLY:C     | 2.45                     | 0.42              |
| 54:CU:89:LEU:HA   | 54:CU:89:LEU:HD23  | 1.79                     | 0.42              |
| 54:CU:160:TYR:CD2 | 54:CU:161:LYS:HG2  | 2.55                     | 0.42              |
| 56:CW:66:ASP:OD1  | 56:CW:67:PRO:HD2   | 2.19                     | 0.42              |
| 59:CZ:45:LEU:CD2  | 78:DS:144:VAL:HG21 | 2.50                     | 0.42              |
| 59:CZ:128:ALA:C   | 59:CZ:133:ARG:HB2  | 2.45                     | 0.42              |
| 70:DK:59:ILE:HD12 | 70:DK:71:CYS:SG    | 2.59                     | 0.42              |
| 78:DS:184:GLY:O   | 78:DS:186:CYS:N    | 2.47                     | 0.42              |
| 81:P0:42:ARG:NH2  | 81:P0:51:VAL:HB    | 2.35                     | 0.42              |
| 1:1:53:C:H5''     | 1:1:1544:C:H1'     | 2.01                     | 0.42              |
| 1:1:143:A:O2'     | 16:v:57:GLN:HG3    | 2.20                     | 0.42              |
| 1:1:200:A:H2'     | 1:1:201:G:C8       | 2.53                     | 0.42              |
| 1:1:560:C:H2'     | 1:1:561:U:C6       | 2.55                     | 0.42              |
| 1:1:595:G:C2      | 1:1:606:A:H1'      | 2.54                     | 0.42              |
| 1:1:798:C:C5      | 29:AB:25:HIS:HB3   | 2.55                     | 0.42              |
| 1:1:1156:C:N3     | 33:AF:46:ARG:NH1   | 2.67                     | 0.42              |
| 1:1:1184:U:OP1    | 1:1:1206:U:O2'     | 2.30                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:1:1832:C:O2'   | 1:1:1838:A:N6      | 2.53                     | 0.42              |
| 1:1:3184:G:H4'   | 1:1:3185:G:H5'     | 2.02                     | 0.42              |
| 2:3:107:A:H2'    | 2:3:108:U:C6       | 2.54                     | 0.42              |
| 7:m:197:LYS:HG2  | 7:m:202:GLY:HA3    | 2.01                     | 0.42              |
| 15:u:126:LYS:HB3 | 15:u:126:LYS:HE3   | 1.73                     | 0.42              |
| 25:7:105:ARG:NH2 | 53:I:151:ASP:HA    | 2.35                     | 0.42              |
| 45:i:64:LEU:HG   | 62:R:119:PHE:O     | 2.20                     | 0.42              |
| 46:B:873:U:H2'   | 46:B:874:U:C6      | 2.54                     | 0.42              |
| 46:B:1016:U:H4'  | 46:B:1017:G:OP2    | 2.19                     | 0.42              |
| 46:B:1283:U:O2'  | 46:B:1284:G:H5'    | 2.18                     | 0.42              |
| 46:B:1336:G:H2'  | 46:B:1337:C:O4'    | 2.19                     | 0.42              |
| 46:B:1668:A:C2   | 46:B:1708:A:C6     | 3.08                     | 0.42              |
| 47:C:183:ARG:HG3 | 47:C:188:ILE:HD12  | 2.02                     | 0.42              |
| 48:D:168:MET:O   | 48:D:172:MET:HG3   | 2.20                     | 0.42              |
| 49:E:168:PRO:HG3 | 56:L:57:ARG:HD3    | 2.02                     | 0.42              |
| 53:I:23:LYS:HD3  | 53:I:41:VAL:O      | 2.20                     | 0.42              |
| 64:T:6:THR:OG1   | 64:T:7:LYS:N       | 2.53                     | 0.42              |
| 65:U:49:LYS:HD3  | 65:U:49:LYS:HA     | 1.75                     | 0.42              |
| 70:Z:54:LEU:HD11 | 70:Z:75:GLN:HB2    | 2.02                     | 0.42              |
| 1:AS:61:A:H5''   | 16:BI:164:LEU:HD21 | 2.01                     | 0.42              |
| 1:AS:430:G:H2'   | 1:AS:431:A:H8      | 1.85                     | 0.42              |
| 1:AS:812:A:H5''  | 1:AS:916:A:H62     | 1.84                     | 0.42              |
| 1:AS:1937:C:O2'  | 1:AS:3309:A:N6     | 2.53                     | 0.42              |
| 1:AS:2254:G:H1   | 1:AS:2288:U:H3     | 1.67                     | 0.42              |
| 1:AS:2356:C:H2'  | 1:AS:2357:U:C6     | 2.54                     | 0.42              |
| 1:AS:2408:A:H2'  | 1:AS:2409:C:C6     | 2.55                     | 0.42              |
| 1:AS:2709:C:OP1  | 22:BO:69:LYS:HE2   | 2.19                     | 0.42              |
| 1:AS:2886:G:H5'' | 5:AX:9:PRO:HG3     | 2.01                     | 0.42              |
| 5:AX:35:ASP:OD2  | 5:AX:191:LYS:NZ    | 2.34                     | 0.42              |
| 5:AX:279:ASN:OD1 | 5:AX:343:TYR:OH    | 2.30                     | 0.42              |
| 6:AY:32:ARG:HG3  | 6:AY:121:TYR:CE1   | 2.54                     | 0.42              |
| 7:AZ:289:LYS:HD2 | 80:BE:206:LEU:HD23 | 2.01                     | 0.42              |
| 14:BG:31:LYS:O   | 14:BG:35:ARG:HB2   | 2.20                     | 0.42              |
| 18:BK:4:TYR:OH   | 18:BK:18:ARG:HG3   | 2.20                     | 0.42              |
| 18:BK:51:VAL:HA  | 18:BK:56:ARG:O     | 2.20                     | 0.42              |
| 23:BP:20:ALA:O   | 23:BP:21:ALA:C     | 2.63                     | 0.42              |
| 23:BP:36:TYR:O   | 23:BP:40:HIS:HB2   | 2.20                     | 0.42              |
| 46:CM:70:C:H2'   | 46:CM:71:A:O4'     | 2.20                     | 0.42              |
| 46:CM:136:U:H6   | 46:CM:136:U:H2'    | 1.66                     | 0.42              |
| 46:CM:1157:G:H2' | 46:CM:1158:C:C6    | 2.55                     | 0.42              |
| 48:CO:51:SER:HB2 | 48:CO:57:ALA:CB    | 2.49                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:CR:93:GLU:H     | 51:CR:93:GLU:HG2  | 1.65                     | 0.42              |
| 52:CS:58:LEU:O     | 52:CS:62:ILE:N    | 2.52                     | 0.42              |
| 56:CW:128:LEU:HD23 | 56:CW:133:HIS:HD2 | 1.85                     | 0.42              |
| 57:CX:93:LYS:HG3   | 57:CX:94:ASN:N    | 2.35                     | 0.42              |
| 79:DT:259:ILE:HD13 | 79:DT:259:ILE:HA  | 1.88                     | 0.42              |
| 1:1:15:A:H2'       | 1:1:16:G:O4'      | 2.20                     | 0.42              |
| 1:1:802:A:N3       | 1:1:2784:C:O2'    | 2.45                     | 0.42              |
| 1:1:1468:U:H2'     | 1:1:1469:G:H8     | 1.85                     | 0.42              |
| 1:1:2126:U:H2'     | 1:1:2127:A:C5     | 2.55                     | 0.42              |
| 1:1:2420:G:H2'     | 1:1:2421:A:H8     | 1.84                     | 0.42              |
| 1:1:2857:C:O2'     | 1:1:2858:U:H5'    | 2.20                     | 0.42              |
| 4:j:5:ILE:HG12     | 4:j:8:GLN:HG3     | 2.01                     | 0.42              |
| 4:j:107:CYS:HB2    | 4:j:136:ILE:HD12  | 2.01                     | 0.42              |
| 4:j:117:GLU:OE2    | 4:j:163:ARG:NE    | 2.52                     | 0.42              |
| 4:j:170:ALA:HB1    | 44:AQ:66:GLY:O    | 2.20                     | 0.42              |
| 6:l:141:HIS:HA     | 6:l:178:ASP:OD1   | 2.20                     | 0.42              |
| 14:t:174:LEU:HD23  | 14:t:174:LEU:HA   | 1.91                     | 0.42              |
| 24:6:80:ARG:NH2    | 24:6:116:GLY:HA3  | 2.35                     | 0.42              |
| 46:B:93:A:O2'      | 51:G:4:GLY:HA3    | 2.20                     | 0.42              |
| 46:B:391:C:H2'     | 46:B:392:C:C6     | 2.55                     | 0.42              |
| 46:B:653:G:O2'     | 46:B:672:U:N3     | 2.22                     | 0.42              |
| 46:B:796:A:N6      | 46:B:843:G:H2'    | 2.35                     | 0.42              |
| 46:B:1334:G:H1'    | 46:B:1365:C:N4    | 2.35                     | 0.42              |
| 46:B:1410:A:C8     | 49:E:87:ALA:HB2   | 2.55                     | 0.42              |
| 46:B:1415:G:H2'    | 46:B:1416:U:O2    | 2.20                     | 0.42              |
| 46:B:1669:U:O2'    | 46:B:1670:U:O5'   | 2.37                     | 0.42              |
| 46:B:1774:C:H2'    | 46:B:1775:G:H8    | 1.84                     | 0.42              |
| 47:C:17:LEU:HD22   | 47:C:22:VAL:HG11  | 2.01                     | 0.42              |
| 52:H:129:PRO:O     | 52:H:133:VAL:HG23 | 2.19                     | 0.42              |
| 56:L:124:HIS:CE1   | 56:L:128:LEU:HD11 | 2.55                     | 0.42              |
| 57:M:47:GLN:O      | 57:M:51:SER:HB3   | 2.19                     | 0.42              |
| 67:W:29:LYS:HE2    | 67:W:110:GLY:HA3  | 2.02                     | 0.42              |
| 78:h:178:LYS:HD2   | 78:h:178:LYS:HA   | 1.93                     | 0.42              |
| 1:AS:21:G:OP1      | 38:CE:43:LYS:HE2  | 2.20                     | 0.42              |
| 1:AS:176:G:C5      | 1:AS:177:C:C5     | 3.08                     | 0.42              |
| 1:AS:491:C:O2'     | 1:AS:620:A:H2     | 2.02                     | 0.42              |
| 1:AS:1905:A:H2'    | 1:AS:1906:A:C8    | 2.55                     | 0.42              |
| 1:AS:1937:C:H2'    | 1:AS:1938:U:C6    | 2.55                     | 0.42              |
| 1:AS:2115:U:C6     | 1:AS:2119:U:C4    | 3.08                     | 0.42              |
| 1:AS:2514:G:C4     | 1:AS:2515:G:N2    | 2.87                     | 0.42              |
| 3:AU:78:G:H2'      | 3:AU:79:A:N3      | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AU:154:C:H5''    | 10:BC:182:LYS:CD   | 2.45                     | 0.42              |
| 9:BB:189:VAL:HG13  | 9:BB:193:PHE:CD2   | 2.55                     | 0.42              |
| 10:BC:73:PRO:HA    | 10:BC:234:TRP:CE3  | 2.55                     | 0.42              |
| 10:BC:107:LYS:O    | 10:BC:111:THR:OG1  | 2.26                     | 0.42              |
| 11:BD:129:HIS:H    | 11:BD:157:ASN:HD21 | 1.66                     | 0.42              |
| 14:BG:54:LEU:HD22  | 14:BG:119:TYR:CG   | 2.55                     | 0.42              |
| 23:BP:22:PRO:HB3   | 23:BP:96:ILE:CD1   | 2.50                     | 0.42              |
| 25:BR:93:ARG:HD2   | 53:CT:156:PHE:HD2  | 1.85                     | 0.42              |
| 29:BV:70:ARG:HD2   | 29:BV:129:PHE:CD2  | 2.55                     | 0.42              |
| 37:CD:33:SER:OG    | 37:CD:36:THR:HG23  | 2.19                     | 0.42              |
| 46:CM:43:A:O2'     | 46:CM:99:C:OP1     | 2.23                     | 0.42              |
| 46:CM:188:U:O4     | 55:CV:143:ARG:HB2  | 2.20                     | 0.42              |
| 46:CM:1187:A:H3'   | 46:CM:1187:A:N3    | 2.34                     | 0.42              |
| 46:CM:1720:C:H2'   | 46:CM:1721:U:H6    | 1.85                     | 0.42              |
| 48:CO:51:SER:HA    | 48:CO:55:LYS:HD2   | 2.02                     | 0.42              |
| 48:CO:182:ALA:HB2  | 48:CO:231:LEU:HD22 | 2.02                     | 0.42              |
| 50:CQ:219:ILE:HD11 | 79:DT:190:ILE:CD1  | 2.47                     | 0.42              |
| 52:CS:120:ILE:HG12 | 72:DM:100:ILE:HG12 | 2.02                     | 0.42              |
| 55:CV:48:THR:HG22  | 55:CV:52:ASN:C     | 2.45                     | 0.42              |
| 57:CX:17:GLN:HA    | 57:CX:89:LEU:H     | 1.85                     | 0.42              |
| 63:DD:42:ILE:H     | 63:DD:42:ILE:HG13  | 1.62                     | 0.42              |
| 79:DT:36:GLY:HA3   | 79:DT:72:VAL:HG21  | 2.01                     | 0.42              |
| 81:P0:59:VAL:HG21  | 81:P0:86:PHE:HZ    | 1.85                     | 0.42              |
| 1:1:561:U:H2'      | 1:1:562:C:C6       | 2.55                     | 0.41              |
| 1:1:2140:U:H2'     | 1:1:2141:C:O4'     | 2.20                     | 0.41              |
| 1:1:2197:A:H2'     | 1:1:2198:A:H8      | 1.86                     | 0.41              |
| 1:1:2656:C:H2'     | 1:1:2657:C:C6      | 2.55                     | 0.41              |
| 1:1:2886:G:H5''    | 5:k:9:PRO:HG3      | 2.00                     | 0.41              |
| 1:1:2890:G:H2'     | 1:1:2891:A:H8      | 1.85                     | 0.41              |
| 1:1:2902:A:H2'     | 1:1:2903:C:H6      | 1.84                     | 0.41              |
| 1:1:3269:C:O2      | 5:k:25:GLN:NE2     | 2.53                     | 0.41              |
| 2:3:69:A:C6        | 2:3:110:G:C6       | 3.08                     | 0.41              |
| 3:4:6:U:H2'        | 3:4:7:U:H6         | 1.84                     | 0.41              |
| 9:o:134:TYR:CZ     | 9:o:228:ASN:HB2    | 2.55                     | 0.41              |
| 13:s:115:LYS:NZ    | 62:R:4:ALA:HB3     | 2.35                     | 0.41              |
| 15:u:17:ARG:HH11   | 15:u:61:VAL:CG2    | 2.33                     | 0.41              |
| 32:AE:45:THR:HG22  | 32:AE:47:ASP:N     | 2.31                     | 0.41              |
| 45:i:126:GLU:O     | 45:i:130:GLU:HG2   | 2.20                     | 0.41              |
| 46:B:521:G:OP2     | 71:a:37:LYS:NZ     | 2.30                     | 0.41              |
| 46:B:938:G:H2'     | 46:B:939:G:H8      | 1.85                     | 0.41              |
| 46:B:1503:A:O2'    | 46:B:1504:U:H5'    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:B:1523:G:H2'    | 46:B:1525:U:C6     | 2.55                     | 0.41              |
| 46:B:1529:G:N2     | 46:B:1555:C:HO2'   | 2.17                     | 0.41              |
| 46:B:1539:U:O2     | 46:B:1584:A:H2     | 2.03                     | 0.41              |
| 51:G:99:PHE:CE1    | 51:G:113:ARG:HG2   | 2.55                     | 0.41              |
| 52:H:148:ARG:HB3   | 52:H:157:ARG:HH11  | 1.85                     | 0.41              |
| 59:O:36:LEU:O      | 59:O:38:HIS:N      | 2.53                     | 0.41              |
| 76:f:15:GLY:H      | 76:f:18:SER:CB     | 2.33                     | 0.41              |
| 78:h:123:LYS:HD3   | 78:h:123:LYS:HA    | 1.89                     | 0.41              |
| 1:AS:412:G:H2'     | 1:AS:413:U:H6      | 1.84                     | 0.41              |
| 1:AS:2204:U:H2'    | 1:AS:2205:C:C6     | 2.55                     | 0.41              |
| 1:AS:2351:A:O2'    | 1:AS:2795:G:N2     | 2.49                     | 0.41              |
| 1:AS:2594:C:H42    | 80:BE:116:ARG:HH12 | 1.68                     | 0.41              |
| 1:AS:2603:U:H4'    | 1:AS:2669:A:H2     | 1.85                     | 0.41              |
| 1:AS:2658:A:H2'    | 1:AS:2659:G:O4'    | 2.20                     | 0.41              |
| 1:AS:2919:G:N3     | 5:AX:250:ALA:HB1   | 2.34                     | 0.41              |
| 1:AS:3157:A:N1     | 21:BN:171:PHE:HB3  | 2.35                     | 0.41              |
| 1:AS:3159:A:C2     | 1:AS:3160:C:C4     | 3.08                     | 0.41              |
| 8:BA:6:PRO:HB3     | 33:BZ:93:TYR:CE1   | 2.54                     | 0.41              |
| 13:BF:32:ARG:NH1   | 13:BF:120:ILE:O    | 2.53                     | 0.41              |
| 14:BG:21:ARG:NH1   | 16:BI:191:TRP:CH2  | 2.88                     | 0.41              |
| 14:BG:35:ARG:O     | 14:BG:39:ARG:HD3   | 2.20                     | 0.41              |
| 17:BJ:131:LYS:HB3  | 17:BJ:134:ARG:HG2  | 2.01                     | 0.41              |
| 23:BP:19:VAL:HA    | 23:BP:108:LEU:CD1  | 2.44                     | 0.41              |
| 27:BT:113:LYS:HB2  | 27:BT:113:LYS:HE2  | 1.87                     | 0.41              |
| 46:CM:809:G:H2'    | 46:CM:810:U:H6     | 1.85                     | 0.41              |
| 46:CM:1668:A:H1'   | 53:CT:66:GLY:HA2   | 2.02                     | 0.41              |
| 48:CO:32:ILE:HA    | 48:CO:96:LEU:O     | 2.21                     | 0.41              |
| 50:CQ:73:LEU:CD2   | 57:CX:20:VAL:HB    | 2.50                     | 0.41              |
| 54:CU:21:PHE:N     | 54:CU:21:PHE:HD1   | 2.18                     | 0.41              |
| 56:CW:126:ARG:HE   | 77:DR:33:ARG:HD3   | 1.84                     | 0.41              |
| 61:DB:53:TYR:CE2   | 61:DB:57:LEU:HD11  | 2.55                     | 0.41              |
| 62:DC:36:LEU:O     | 62:DC:37:CYS:HB3   | 2.19                     | 0.41              |
| 63:DD:93:GLN:HE21  | 79:DT:61:SER:HB2   | 1.84                     | 0.41              |
| 66:DG:111:ILE:HG23 | 66:DG:113:VAL:HG23 | 2.02                     | 0.41              |
| 74:DO:10:PRO:HD2   | 74:DO:24:LEU:HD11  | 2.02                     | 0.41              |
| 79:DT:21:THR:HB    | 79:DT:70:GLN:HA    | 2.01                     | 0.41              |
| 79:DT:41:THR:CG2   | 79:DT:42:LEU:N     | 2.83                     | 0.41              |
| 79:DT:103:ARG:HE   | 79:DT:105:VAL:HG21 | 1.82                     | 0.41              |
| 79:DT:152:VAL:HA   | 79:DT:170:SER:HB2  | 2.00                     | 0.41              |
| 82:12:137:GLN:O    | 82:12:138:SER:C    | 2.63                     | 0.41              |
| 1:1:29:G:C6        | 1:1:54:G:C6        | 3.08                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1:243:G:H1'     | 14:BG:131:LYS:NZ   | 2.35                     | 0.41              |
| 1:1:2985:U:H2'    | 1:1:2986:U:C6      | 2.54                     | 0.41              |
| 1:1:3234:U:H3     | 8:n:134:ARG:HH11   | 1.67                     | 0.41              |
| 1:1:3285:A:H4'    | 5:k:174:LYS:NZ     | 2.34                     | 0.41              |
| 3:4:149:A:H2'     | 3:4:150:G:C8       | 2.55                     | 0.41              |
| 11:q:41:ILE:HG22  | 11:q:43:VAL:HG13   | 2.01                     | 0.41              |
| 14:t:56:PRO:HG3   | 14:t:74:GLY:C      | 2.45                     | 0.41              |
| 16:v:151:ILE:HD12 | 16:v:156:HIS:HB3   | 2.01                     | 0.41              |
| 20:z:72:ALA:O     | 20:z:74:ARG:NH1    | 2.53                     | 0.41              |
| 25:7:98:PRO:HA    | 25:7:101:ARG:HB2   | 2.01                     | 0.41              |
| 46:B:372:U:O2'    | 46:B:601:U:OP1     | 2.32                     | 0.41              |
| 46:B:586:U:H2'    | 46:B:587:C:H6      | 1.85                     | 0.41              |
| 46:B:608:G:O2'    | 46:B:611:G:O3'     | 2.38                     | 0.41              |
| 46:B:652:C:N4     | 46:B:654:G:C4      | 2.88                     | 0.41              |
| 46:B:1187:A:H1'   | 46:B:1192:C:N4     | 2.35                     | 0.41              |
| 46:B:1258:G:N7    | 46:B:1416:U:H3'    | 2.35                     | 0.41              |
| 46:B:1312:C:C2    | 46:B:1313:G:C8     | 3.07                     | 0.41              |
| 50:F:219:ILE:O    | 79:AR:191:GLY:HA2  | 2.20                     | 0.41              |
| 54:J:24:LEU:HD11  | 54:J:76:GLU:HB3    | 2.02                     | 0.41              |
| 62:R:50:ASP:OD1   | 62:R:50:ASP:N      | 2.53                     | 0.41              |
| 71:a:20:ARG:HB3   | 71:a:76:TYR:CD2    | 2.54                     | 0.41              |
| 1:AS:38:A:H2'     | 1:AS:41:C:N4       | 2.35                     | 0.41              |
| 1:AS:637:G:OP1    | 33:BZ:41:SER:HB2   | 2.19                     | 0.41              |
| 1:AS:733:A:H8     | 1:AS:733:A:OP2     | 2.04                     | 0.41              |
| 1:AS:3014:U:O3'   | 24:BQ:45:ARG:HD3   | 2.20                     | 0.41              |
| 14:BG:154:PRO:HB2 | 14:BG:155:GLU:H    | 1.68                     | 0.41              |
| 24:BQ:84:PRO:HA   | 24:BQ:93:LEU:O     | 2.20                     | 0.41              |
| 25:BR:89:LEU:O    | 25:BR:92:GLU:HG2   | 2.20                     | 0.41              |
| 27:BT:37:LYS:NZ   | 27:BT:40:ARG:HH11  | 2.19                     | 0.41              |
| 33:BZ:33:TRP:HH2  | 33:BZ:53:GLN:HG2   | 1.85                     | 0.41              |
| 33:BZ:98:ALA:HB3  | 33:BZ:101:VAL:HG23 | 2.01                     | 0.41              |
| 38:CE:52:LYS:HE2  | 38:CE:55:ARG:HH21  | 1.84                     | 0.41              |
| 45:CL:91:HIS:O    | 46:CM:1259:C:N4    | 2.41                     | 0.41              |
| 46:CM:121:U:H2'   | 46:CM:122:U:C6     | 2.55                     | 0.41              |
| 46:CM:653:G:O2'   | 46:CM:655:U:C4     | 2.73                     | 0.41              |
| 46:CM:671:G:N2    | 46:CM:672:U:O2     | 2.52                     | 0.41              |
| 46:CM:839:U:O4    | 46:CM:840:A:N6     | 2.53                     | 0.41              |
| 46:CM:1339:G:O6   | 46:CM:1354:U:C2    | 2.73                     | 0.41              |
| 46:CM:1609:G:H2'  | 46:CM:1610:C:H6    | 1.85                     | 0.41              |
| 46:CM:1623:C:O2   | 46:CM:1752:A:N6    | 2.53                     | 0.41              |
| 46:CM:1742:A:O2'  | 46:CM:1743:A:C8    | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:CS:159:ALA:O   | 75:DP:61:ARG:NH2  | 2.53                     | 0.41              |
| 59:CZ:69:GLU:O    | 59:CZ:70:SER:C    | 2.63                     | 0.41              |
| 64:DE:85:VAL:HA   | 64:DE:86:PRO:HD3  | 1.94                     | 0.41              |
| 79:DT:101:THR:CG2 | 79:DT:102:GLN:H   | 2.32                     | 0.41              |
| 1:1:95:G:H2'      | 1:1:96:U:O4'      | 2.20                     | 0.41              |
| 1:1:812:A:H5''    | 1:1:916:A:H62     | 1.84                     | 0.41              |
| 1:1:988:A:H61     | 1:1:1053:A:H61    | 1.69                     | 0.41              |
| 1:1:1209:G:O2'    | 21:0:90:MET:HE2   | 2.20                     | 0.41              |
| 1:1:1239:G:OP2    | 1:1:1239:G:H8     | 2.04                     | 0.41              |
| 1:1:1278:G:OP1    | 81:P0:56:ASN:N    | 2.45                     | 0.41              |
| 1:1:1400:G:N1     | 1:1:1404:A:C6     | 2.88                     | 0.41              |
| 1:1:1805:A:H2'    | 1:1:1806:A:O4'    | 2.20                     | 0.41              |
| 1:1:1813:G:H2'    | 1:1:1814:U:H5'    | 2.02                     | 0.41              |
| 1:1:2236:U:H2'    | 1:1:2237:A:H8     | 1.85                     | 0.41              |
| 1:1:2260:U:O2     | 1:1:2288:U:H4'    | 2.20                     | 0.41              |
| 1:1:2445:G:N2     | 1:1:2467:C:H1'    | 2.35                     | 0.41              |
| 1:1:2583:U:H2'    | 1:1:2584:U:H6     | 1.84                     | 0.41              |
| 1:1:2606:U:C2     | 1:1:2617:G:C6     | 3.07                     | 0.41              |
| 1:1:2849:G:H2'    | 1:1:2850:G:C8     | 2.55                     | 0.41              |
| 1:1:2967:A:H2'    | 1:1:2968:U:O4'    | 2.21                     | 0.41              |
| 4:j:77:ILE:CD1    | 4:j:128:ARG:HB3   | 2.48                     | 0.41              |
| 13:s:53:THR:HG23  | 13:s:60:ARG:HA    | 2.02                     | 0.41              |
| 14:t:167:THR:HB   | 29:AB:135:GLU:OE1 | 2.20                     | 0.41              |
| 18:x:116:HIS:HB3  | 18:x:149:THR:HB   | 2.02                     | 0.41              |
| 38:AK:39:TYR:CD1  | 38:AK:40:PRO:HA   | 2.55                     | 0.41              |
| 46:B:182:C:H2'    | 46:B:183:C:C6     | 2.56                     | 0.41              |
| 46:B:394:G:N2     | 46:B:396:G:H3'    | 2.35                     | 0.41              |
| 46:B:509:A:H5'    | 56:L:173:LYS:HB2  | 2.02                     | 0.41              |
| 46:B:597:A:H2'    | 46:B:598:U:C6     | 2.54                     | 0.41              |
| 46:B:806:A:H3'    | 46:B:806:A:OP1    | 2.20                     | 0.41              |
| 46:B:883:A:N3     | 46:B:884:G:H1'    | 2.35                     | 0.41              |
| 46:B:974:U:H2'    | 46:B:975:C:C6     | 2.54                     | 0.41              |
| 46:B:1342:A:C6    | 46:B:1352:G:C6    | 3.09                     | 0.41              |
| 46:B:1378:U:H2'   | 46:B:1379:C:C6    | 2.55                     | 0.41              |
| 46:B:1763:A:H2'   | 46:B:1764:G:C8    | 2.55                     | 0.41              |
| 47:C:201:LEU:O    | 47:C:202:TYR:HB2  | 2.20                     | 0.41              |
| 52:H:63:GLN:OE1   | 52:H:88:PRO:HA    | 2.20                     | 0.41              |
| 52:H:63:GLN:HE22  | 52:H:66:ASN:HB2   | 1.85                     | 0.41              |
| 54:J:25:GLU:HA    | 54:J:30:LEU:O     | 2.20                     | 0.41              |
| 57:M:59:PHE:CZ    | 57:M:62:GLN:HA    | 2.56                     | 0.41              |
| 63:S:28:ILE:HG22  | 63:S:35:ILE:HG21  | 2.00                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:b:84:GLU:OE1    | 72:b:94:LYS:NZ     | 2.54                     | 0.41              |
| 78:h:182:TYR:CE1   | 78:h:187:HIS:HA    | 2.54                     | 0.41              |
| 1:AS:97:G:H4'      | 1:AS:281:G:OP1     | 2.20                     | 0.41              |
| 1:AS:794:G:H2'     | 1:AS:795:G:O4'     | 2.20                     | 0.41              |
| 1:AS:797:A:OP1     | 29:BV:27:LYS:HE3   | 2.20                     | 0.41              |
| 1:AS:875:U:O2'     | 18:BK:131:ARG:HD2  | 2.20                     | 0.41              |
| 1:AS:1452:A:N1     | 32:BY:63:VAL:HB    | 2.36                     | 0.41              |
| 1:AS:2960:C:OP1    | 17:BJ:69:LYS:HE3   | 2.20                     | 0.41              |
| 83:AS:3401:3K5:H21 | 43:CJ:43:TYR:CE2   | 2.54                     | 0.41              |
| 6:AY:189:ARG:NE    | 6:AY:198:ARG:O     | 2.48                     | 0.41              |
| 16:BI:47:LYS:HE3   | 16:BI:51:LEU:HD11  | 2.02                     | 0.41              |
| 18:BK:112:LEU:HD13 | 18:BK:150:LEU:HD13 | 2.02                     | 0.41              |
| 19:BL:76:ALA:HA    | 19:BL:79:LYS:HG3   | 2.02                     | 0.41              |
| 23:BP:78:TYR:HD1   | 23:BP:78:TYR:O     | 2.03                     | 0.41              |
| 25:BR:6:ASP:HA     | 25:BR:13:ILE:HD11  | 2.02                     | 0.41              |
| 30:BW:28:LYS:HG2   | 30:BW:29:TYR:CD1   | 2.55                     | 0.41              |
| 39:CF:30:LYS:HB3   | 39:CF:38:PHE:CD2   | 2.55                     | 0.41              |
| 46:CM:205:U:H2'    | 46:CM:206:U:C6     | 2.55                     | 0.41              |
| 46:CM:764:U:C2     | 71:DL:8:ARG:HD3    | 2.55                     | 0.41              |
| 46:CM:770:C:P      | 46:CM:770:C:O4'    | 2.78                     | 0.41              |
| 46:CM:1414:G:C2'   | 46:CM:1415:G:H5'   | 2.50                     | 0.41              |
| 47:CN:3:LEU:HD22   | 47:CN:62:ARG:HH22  | 1.85                     | 0.41              |
| 47:CN:21:ASN:HB3   | 47:CN:24:LEU:HD12  | 2.02                     | 0.41              |
| 47:CN:107:PHE:HD2  | 47:CN:135:GLU:HB2  | 1.85                     | 0.41              |
| 47:CN:110:TYR:HA   | 47:CN:115:PHE:CD1  | 2.55                     | 0.41              |
| 51:CR:58:GLY:HA2   | 51:CR:61:VAL:HG12  | 2.02                     | 0.41              |
| 52:CS:43:PHE:CD2   | 52:CS:115:LYS:HD3  | 2.55                     | 0.41              |
| 52:CS:159:ALA:HB2  | 52:CS:225:ARG:HG2  | 2.01                     | 0.41              |
| 53:CT:136:LYS:HG3  | 53:CT:173:PRO:HB2  | 2.01                     | 0.41              |
| 61:DB:27:ASP:OD1   | 61:DB:30:GLY:N     | 2.50                     | 0.41              |
| 61:DB:98:ARG:HD2   | 73:DN:49:ALA:HB2   | 2.01                     | 0.41              |
| 79:DT:22:SER:HB3   | 79:DT:71:ASP:HA    | 2.01                     | 0.41              |
| 79:DT:75:SER:C     | 79:DT:77:ASP:N     | 2.77                     | 0.41              |
| 79:DT:128:ARG:HG2  | 79:DT:151:TRP:CG   | 2.54                     | 0.41              |
| 79:DT:283:ASP:O    | 79:DT:284:PRO:C    | 2.63                     | 0.41              |
| 1:1:79:G:H2'       | 1:1:80:C:C6        | 2.55                     | 0.41              |
| 1:1:122:A:C6       | 1:1:149:A:C5       | 3.09                     | 0.41              |
| 1:1:725:G:H2'      | 1:1:726:G:O4'      | 2.20                     | 0.41              |
| 1:1:819:C:H5'      | 4:j:19:HIS:CD2     | 2.55                     | 0.41              |
| 1:1:1093:G:H2'     | 1:1:1093:G:N3      | 2.36                     | 0.41              |
| 1:1:1215:C:OP2     | 81:P0:5:ARG:NH2    | 2.53                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1:1579:A:H2'     | 1:1:1580:U:O4'     | 2.20                     | 0.41              |
| 1:1:1611:U:H5''    | 35:AH:64:GLN:OE1   | 2.19                     | 0.41              |
| 1:1:3037:G:H2'     | 1:1:3038:U:C6      | 2.55                     | 0.41              |
| 1:1:3039:C:H5''    | 20:z:58:HIS:NE2    | 2.36                     | 0.41              |
| 1:1:3316:U:OP1     | 55:K:124:LYS:NZ    | 2.44                     | 0.41              |
| 3:4:7:U:H2'        | 3:4:8:C:C6         | 2.55                     | 0.41              |
| 3:4:12:A:C6        | 3:4:13:A:N7        | 2.88                     | 0.41              |
| 9:o:78:GLN:HB2     | 22:2:135:PRO:HB2   | 2.02                     | 0.41              |
| 10:p:69:ARG:HD3    | 10:p:238:ILE:O     | 2.21                     | 0.41              |
| 10:p:254:ALA:O     | 10:p:258:VAL:HG12  | 2.19                     | 0.41              |
| 12:r:48:LEU:HD21   | 12:r:145:LYS:HG3   | 2.02                     | 0.41              |
| 13:s:21:ILE:HD11   | 13:s:125:MET:HE2   | 2.02                     | 0.41              |
| 14:t:131:LYS:H     | 14:t:131:LYS:HG2   | 1.46                     | 0.41              |
| 45:i:96:LYS:HB2    | 45:i:96:LYS:HE3    | 1.70                     | 0.41              |
| 46:B:167:A:OP1     | 53:I:137:ARG:NE    | 2.53                     | 0.41              |
| 46:B:279:G:H8      | 46:B:279:G:P       | 2.43                     | 0.41              |
| 46:B:988:A:H2'     | 46:B:990:A:N7      | 2.35                     | 0.41              |
| 46:B:1575:G:H5'    | 46:B:1576:C:OP2    | 2.20                     | 0.41              |
| 46:B:1743:A:OP2    | 86:B:1851:GET:O41  | 2.35                     | 0.41              |
| 51:G:59:ARG:NH1    | 71:a:87:PRO:HG3    | 2.35                     | 0.41              |
| 53:I:196:LYS:O     | 53:I:200:GLN:HG2   | 2.20                     | 0.41              |
| 56:L:37:LYS:HA     | 77:g:33:ARG:HA     | 2.01                     | 0.41              |
| 60:P:46:THR:HG21   | 60:P:90:TYR:HE2    | 1.84                     | 0.41              |
| 79:AR:145:LEU:HA   | 79:AR:145:LEU:HD23 | 1.83                     | 0.41              |
| 79:AR:200:THR:HG21 | 79:AR:242:PHE:H    | 1.85                     | 0.41              |
| 1:AS:270:U:H2'     | 1:AS:271:C:C6      | 2.56                     | 0.41              |
| 1:AS:1050:A:H5''   | 1:AS:2609:A:H61    | 1.84                     | 0.41              |
| 1:AS:1911:A:H2'    | 1:AS:1912:U:H6     | 1.84                     | 0.41              |
| 1:AS:2322:U:H2'    | 1:AS:2323:A:H8     | 1.85                     | 0.41              |
| 1:AS:3038:U:H2'    | 1:AS:3039:C:H6     | 1.85                     | 0.41              |
| 1:AS:3146:G:N2     | 1:AS:3178:A:H1'    | 2.35                     | 0.41              |
| 1:AS:3204:G:H2'    | 1:AS:3205:C:C6     | 2.55                     | 0.41              |
| 2:AT:44:C:OP2      | 13:BF:137:ARG:NH1  | 2.35                     | 0.41              |
| 4:AW:27:ALA:HB1    | 4:AW:77:ILE:HG13   | 2.02                     | 0.41              |
| 6:AY:153:VAL:CG1   | 6:AY:173:VAL:HG11  | 2.50                     | 0.41              |
| 6:AY:236:LEU:HD12  | 6:AY:236:LEU:HA    | 1.89                     | 0.41              |
| 9:BB:134:TYR:HA    | 9:BB:233:ILE:HD12  | 2.02                     | 0.41              |
| 80:BE:31:ILE:HA    | 80:BE:66:GLU:OE1   | 2.19                     | 0.41              |
| 13:BF:160:ILE:HG23 | 13:BF:171:VAL:HG21 | 2.01                     | 0.41              |
| 14:BG:61:PRO:C     | 14:BG:62:THR:HG23  | 2.46                     | 0.41              |
| 36:CC:104:ALA:O    | 36:CC:108:ARG:HB2  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:CD:36:THR:O    | 37:CD:40:ARG:HD2  | 2.20                     | 0.41              |
| 46:CM:7:G:H4'     | 46:CM:571:C:H4'   | 2.01                     | 0.41              |
| 46:CM:151:G:H2'   | 46:CM:152:G:H8    | 1.84                     | 0.41              |
| 46:CM:803:G:C4    | 46:CM:838:G:N2    | 2.89                     | 0.41              |
| 46:CM:840:A:O2'   | 46:CM:841:A:H3'   | 2.20                     | 0.41              |
| 46:CM:1086:G:N2   | 69:DJ:2:THR:O     | 2.53                     | 0.41              |
| 46:CM:1335:U:O2'  | 46:CM:1336:G:OP1  | 2.34                     | 0.41              |
| 46:CM:1349:G:N2   | 66:DG:3:GLY:HA3   | 2.35                     | 0.41              |
| 46:CM:1369:G:H5'' | 67:DH:88:ARG:HH21 | 1.85                     | 0.41              |
| 46:CM:1520:C:H4'  | 46:CM:1526:G:C6   | 2.55                     | 0.41              |
| 46:CM:1555:C:H4'  | 46:CM:1556:A:O5'  | 2.21                     | 0.41              |
| 50:CQ:178:MET:HG3 | 50:CQ:183:LEU:CD2 | 2.50                     | 0.41              |
| 52:CS:139:ASN:C   | 52:CS:214:LYS:NZ  | 2.79                     | 0.41              |
| 55:CV:106:ALA:HB2 | 55:CV:171:LEU:HG  | 2.02                     | 0.41              |
| 78:DS:188:LEU:HG  | 78:DS:190:LEU:H   | 1.85                     | 0.41              |
| 79:DT:79:ALA:O    | 79:DT:95:LEU:HD23 | 2.20                     | 0.41              |
| 1:1:803:A:H61     | 1:1:930:G:H22     | 1.67                     | 0.41              |
| 1:1:1011:C:O2'    | 1:1:1012:U:P      | 2.78                     | 0.41              |
| 1:1:1083:G:OP1    | 30:AC:29:TYR:OH   | 2.21                     | 0.41              |
| 1:1:1802:A:OP1    | 35:AH:75:ALA:HA   | 2.20                     | 0.41              |
| 1:1:1851:U:H2'    | 1:1:1852:C:C6     | 2.55                     | 0.41              |
| 1:1:2507:A:H2'    | 1:1:2508:G:O4'    | 2.21                     | 0.41              |
| 2:3:60:G:H2'      | 2:3:61:C:H6       | 1.85                     | 0.41              |
| 2:3:98:C:OP1      | 21:0:39:SER:OG    | 2.30                     | 0.41              |
| 7:m:160:PHE:CE2   | 7:m:179:ARG:HB3   | 2.56                     | 0.41              |
| 14:t:143:VAL:HG13 | 14:t:147:PHE:HD2  | 1.85                     | 0.41              |
| 22:2:92:ARG:HB3   | 22:2:94:GLU:OE1   | 2.21                     | 0.41              |
| 25:7:101:ARG:C    | 25:7:103:ALA:H    | 2.29                     | 0.41              |
| 25:7:120:LYS:HB2  | 25:7:120:LYS:HE2  | 1.95                     | 0.41              |
| 25:7:128:ALA:HA   | 25:7:131:VAL:HG12 | 2.02                     | 0.41              |
| 45:i:101:LYS:HB3  | 46:B:573:C:H5''   | 2.02                     | 0.41              |
| 46:B:53:G:H2'     | 46:B:54:C:C6      | 2.55                     | 0.41              |
| 46:B:1553:U:N3    | 46:B:1554:U:C5    | 2.89                     | 0.41              |
| 46:B:1573:A:HO2'  | 46:B:1574:A:P     | 2.42                     | 0.41              |
| 46:B:1720:C:H2'   | 46:B:1721:U:H6    | 1.84                     | 0.41              |
| 47:C:110:TYR:HA   | 47:C:115:PHE:CD1  | 2.56                     | 0.41              |
| 54:J:38:GLN:O     | 54:J:66:TYR:OH    | 2.35                     | 0.41              |
| 54:J:67:ARG:HD3   | 54:J:67:ARG:HA    | 1.82                     | 0.41              |
| 55:K:62:THR:HG22  | 55:K:77:ARG:HA    | 2.03                     | 0.41              |
| 59:O:133:ARG:NH2  | 59:O:136:LEU:HB3  | 2.36                     | 0.41              |
| 67:W:16:GLN:CD    | 67:W:19:HIS:HE2   | 2.24                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:Z:90:ASP:OD1    | 77:g:12:GLY:HA2    | 2.21                     | 0.41              |
| 70:Z:130:VAL:HG21  | 70:Z:143:PRO:HD3   | 2.03                     | 0.41              |
| 79:AR:88:ARG:HA    | 79:AR:111:VAL:HG23 | 2.03                     | 0.41              |
| 1:AS:236:A:H2'     | 1:AS:237:U:O4'     | 2.20                     | 0.41              |
| 1:AS:371:G:H4'     | 1:AS:396:A:N1      | 2.36                     | 0.41              |
| 1:AS:489:G:C2      | 1:AS:490:G:C8      | 3.08                     | 0.41              |
| 1:AS:903:G:H2'     | 1:AS:922:A:H62     | 1.85                     | 0.41              |
| 1:AS:1128:C:H2'    | 1:AS:1129:A:H8     | 1.86                     | 0.41              |
| 1:AS:1852:C:C2     | 1:AS:1853:C:C5     | 3.09                     | 0.41              |
| 1:AS:2330:A:H2'    | 1:AS:2331:G:C8     | 2.55                     | 0.41              |
| 1:AS:2516:U:O2'    | 1:AS:2520:A:N1     | 2.53                     | 0.41              |
| 1:AS:3045:A:H2'    | 1:AS:3046:G:O4'    | 2.21                     | 0.41              |
| 10:BC:134:LYS:HB3  | 10:BC:139:HIS:CE1  | 2.55                     | 0.41              |
| 23:BP:14:LYS:H     | 23:BP:14:LYS:HG2   | 1.72                     | 0.41              |
| 23:BP:107:LYS:O    | 23:BP:108:LEU:HG   | 2.19                     | 0.41              |
| 25:BR:121:ALA:HA   | 25:BR:124:LYS:HD2  | 2.02                     | 0.41              |
| 38:CE:26:SER:HB3   | 38:CE:35:SER:OG    | 2.21                     | 0.41              |
| 45:CL:62:ALA:O     | 45:CL:66:ASN:HB2   | 2.20                     | 0.41              |
| 46:CM:91:G:H2'     | 46:CM:92:A:O4'     | 2.20                     | 0.41              |
| 46:CM:279:G:H2'    | 46:CM:280:C:C6     | 2.55                     | 0.41              |
| 46:CM:444:A:C6     | 46:CM:445:U:C4     | 3.09                     | 0.41              |
| 46:CM:597:A:H2'    | 46:CM:598:U:C6     | 2.56                     | 0.41              |
| 46:CM:680:C:O2'    | 46:CM:681:C:H5''   | 2.21                     | 0.41              |
| 46:CM:1214:G:O6    | 59:CZ:46:ARG:HB3   | 2.20                     | 0.41              |
| 48:CO:31:ASP:HA    | 48:CO:45:LYS:HB2   | 2.03                     | 0.41              |
| 48:CO:79:HIS:C     | 48:CO:81:TYR:H     | 2.29                     | 0.41              |
| 48:CO:164:VAL:O    | 48:CO:168:MET:HG3  | 2.20                     | 0.41              |
| 50:CQ:139:ILE:HG23 | 50:CQ:185:ILE:HG22 | 2.02                     | 0.41              |
| 52:CS:26:ALA:CB    | 63:DD:25:LYS:HB2   | 2.49                     | 0.41              |
| 53:CT:131:LYS:H    | 53:CT:131:LYS:HG2  | 1.37                     | 0.41              |
| 53:CT:161:GLU:O    | 53:CT:161:GLU:HG3  | 2.20                     | 0.41              |
| 59:CZ:62:LEU:O     | 59:CZ:91:VAL:HG12  | 2.20                     | 0.41              |
| 62:DC:17:PHE:O     | 62:DC:18:LYS:C     | 2.64                     | 0.41              |
| 66:DG:6:VAL:HG11   | 66:DG:63:ARG:HG3   | 2.02                     | 0.41              |
| 69:DJ:88:ARG:HG2   | 69:DJ:92:ASN:HD21  | 1.85                     | 0.41              |
| 69:DJ:106:THR:HG23 | 69:DJ:108:ALA:H    | 1.85                     | 0.41              |
| 79:DT:37:SER:HB3   | 79:DT:39:ASP:OD1   | 2.20                     | 0.41              |
| 79:DT:200:THR:O    | 79:DT:209:ALA:N    | 2.53                     | 0.41              |
| 79:DT:289:LEU:HD23 | 79:DT:289:LEU:N    | 2.35                     | 0.41              |
| 1:1:277:G:H2'      | 1:1:278:U:H6       | 1.86                     | 0.41              |
| 1:1:377:A:H1'      | 1:1:392:G:C2       | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:564:G:H2'     | 1:1:565:A:H8      | 1.78                     | 0.41              |
| 1:1:883:G:H2'     | 1:1:884:A:C8      | 2.56                     | 0.41              |
| 1:1:1330:U:H2'    | 1:1:1331:U:C6     | 2.55                     | 0.41              |
| 1:1:1528:C:H2'    | 1:1:1529:U:C6     | 2.56                     | 0.41              |
| 1:1:1932:A:C5'    | 46:B:1655:G:H5'   | 2.50                     | 0.41              |
| 1:1:2603:U:H2'    | 1:1:2604:G:C8     | 2.55                     | 0.41              |
| 4:j:35:ALA:HA     | 10:p:37:ILE:HD13  | 2.02                     | 0.41              |
| 15:u:17:ARG:HH11  | 15:u:61:VAL:HG22  | 1.84                     | 0.41              |
| 16:v:120:TRP:NE1  | 16:v:123:GLN:HE21 | 2.19                     | 0.41              |
| 18:x:30:ARG:NH2   | 18:x:34:GLN:HG3   | 2.36                     | 0.41              |
| 36:AI:105:ARG:HG3 | 36:AI:108:ARG:NH2 | 2.35                     | 0.41              |
| 45:i:73:VAL:O     | 45:i:74:ALA:C     | 2.63                     | 0.41              |
| 46:B:160:A:H2'    | 46:B:161:G:N3     | 2.35                     | 0.41              |
| 46:B:393:U:H2'    | 46:B:394:G:O4'    | 2.21                     | 0.41              |
| 46:B:1337:C:H2'   | 46:B:1338:U:O4'   | 2.21                     | 0.41              |
| 49:E:44:LYS:HD3   | 49:E:44:LYS:HA    | 1.77                     | 0.41              |
| 51:G:196:VAL:CG2  | 51:G:211:LYS:HB2  | 2.50                     | 0.41              |
| 53:I:56:ASN:HB2   | 53:I:108:VAL:HG12 | 2.03                     | 0.41              |
| 60:P:45:LEU:HA    | 60:P:49:GLN:OE1   | 2.20                     | 0.41              |
| 66:V:35:ASP:OD1   | 66:V:35:ASP:N     | 2.42                     | 0.41              |
| 66:V:62:ALA:HB2   | 66:V:108:LEU:HD21 | 2.01                     | 0.41              |
| 1:AS:776:A:C2     | 19:BL:168:LYS:HG3 | 2.55                     | 0.41              |
| 1:AS:892:A:H5'    | 4:AW:183:GLY:HA2  | 2.02                     | 0.41              |
| 1:AS:1099:A:H2'   | 1:AS:1099:A:N3    | 2.36                     | 0.41              |
| 1:AS:1503:G:H1'   | 18:BK:139:TYR:CE2 | 2.55                     | 0.41              |
| 1:AS:1505:A:H2'   | 1:AS:1506:G:C8    | 2.55                     | 0.41              |
| 1:AS:2668:A:H8    | 1:AS:2668:A:OP1   | 2.03                     | 0.41              |
| 1:AS:2919:G:C2    | 5:AX:250:ALA:HB1  | 2.55                     | 0.41              |
| 1:AS:3060:G:OP1   | 5:AX:313:ARG:NH1  | 2.54                     | 0.41              |
| 4:AW:67:TYR:C     | 10:BC:41:ILE:HG23 | 2.46                     | 0.41              |
| 5:AX:140:ASP:OD1  | 5:AX:142:LYS:HD3  | 2.21                     | 0.41              |
| 9:BB:107:THR:HB   | 19:BL:4:ASP:O     | 2.21                     | 0.41              |
| 9:BB:119:LYS:N    | 22:BO:133:ALA:O   | 2.52                     | 0.41              |
| 14:BG:27:ASP:O    | 14:BG:31:LYS:HB2  | 2.20                     | 0.41              |
| 16:BI:101:THR:O   | 16:BI:105:ARG:HD2 | 2.20                     | 0.41              |
| 25:BR:93:ARG:HH12 | 53:CT:156:PHE:HA  | 1.86                     | 0.41              |
| 28:BU:53:VAL:HA   | 28:BU:57:MET:SD   | 2.60                     | 0.41              |
| 29:BV:27:LYS:HA   | 29:BV:27:LYS:HD2  | 1.79                     | 0.41              |
| 37:CD:50:ALA:O    | 37:CD:54:ARG:HG2  | 2.20                     | 0.41              |
| 42:CI:18:ARG:NH1  | 46:CM:1110:A:OP1  | 2.52                     | 0.41              |
| 46:CM:217:A:O5'   | 46:CM:816:U:O2'   | 2.28                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:218:A:H5''   | 46:CM:218:A:C8     | 2.51                     | 0.41              |
| 46:CM:331:A:H2'    | 46:CM:332:G:C8     | 2.56                     | 0.41              |
| 46:CM:463:G:C6     | 46:CM:464:U:C4     | 3.09                     | 0.41              |
| 46:CM:470:U:H5''   | 56:CW:11:THR:HG23  | 2.02                     | 0.41              |
| 46:CM:598:U:H2'    | 46:CM:599:A:C8     | 2.56                     | 0.41              |
| 46:CM:824:U:C5     | 46:CM:825:U:H5     | 2.39                     | 0.41              |
| 46:CM:1126:G:H2'   | 46:CM:1127:A:C8    | 2.55                     | 0.41              |
| 46:CM:1378:U:H2'   | 46:CM:1379:C:H6    | 1.86                     | 0.41              |
| 48:CO:125:VAL:O    | 48:CO:136:ARG:HA   | 2.21                     | 0.41              |
| 52:CS:162:VAL:HG13 | 52:CS:166:ARG:HD3  | 2.02                     | 0.41              |
| 52:CS:181:GLU:O    | 52:CS:182:ALA:C    | 2.64                     | 0.41              |
| 53:CT:234:LEU:HG   | 53:CT:235:LYS:CE   | 2.50                     | 0.41              |
| 59:CZ:105:GLN:OE1  | 59:CZ:113:ARG:C    | 2.63                     | 0.41              |
| 63:DD:96:VAL:HG12  | 63:DD:97:ASP:N     | 2.35                     | 0.41              |
| 74:DO:32:PHE:CZ    | 74:DO:47:PHE:HD1   | 2.38                     | 0.41              |
| 79:DT:6:VAL:HG23   | 79:DT:313:MET:HB3  | 2.01                     | 0.41              |
| 79:DT:161:ASP:O    | 79:DT:163:SER:N    | 2.54                     | 0.41              |
| 79:DT:163:SER:OG   | 79:DT:165:THR:HG23 | 2.21                     | 0.41              |
| 1:1:278:U:OP2      | 43:AP:49:GLY:HA3   | 2.21                     | 0.41              |
| 1:1:480:G:C4       | 1:1:481:G:C8       | 3.09                     | 0.41              |
| 1:1:635:C:C2       | 1:1:636:C:C5       | 3.09                     | 0.41              |
| 1:1:1153:G:H4'     | 1:1:1165:A:O2'     | 2.20                     | 0.41              |
| 1:1:1690:U:O2'     | 1:1:1691:U:H5'     | 2.20                     | 0.41              |
| 1:1:1718:U:OP2     | 20:z:103:ARG:NH1   | 2.48                     | 0.41              |
| 1:1:2173:C:H5''    | 46:B:979:G:O2'     | 2.20                     | 0.41              |
| 1:1:2242:U:H2'     | 1:1:2243:C:H6      | 1.86                     | 0.41              |
| 1:1:2485:U:H2'     | 1:1:2486:U:C6      | 2.56                     | 0.41              |
| 1:1:2557:G:C6      | 26:8:24:LEU:HD21   | 2.56                     | 0.41              |
| 1:1:2619:A:O3'     | 12:r:24:ARG:NH2    | 2.52                     | 0.41              |
| 1:1:2735:U:C4      | 1:1:2736:C:C5      | 3.08                     | 0.41              |
| 1:1:2749:G:H5''    | 1:1:2750:G:OP1     | 2.21                     | 0.41              |
| 1:1:3045:A:H2'     | 1:1:3046:G:O4'     | 2.20                     | 0.41              |
| 1:1:3313:G:H2'     | 1:1:3314:C:H6      | 1.86                     | 0.41              |
| 2:3:1:G:C2         | 2:3:2:G:C8         | 3.09                     | 0.41              |
| 2:3:24:A:H2'       | 2:3:25:G:C8        | 2.56                     | 0.41              |
| 3:4:152:G:H2'      | 3:4:153:U:O4'      | 2.21                     | 0.41              |
| 5:k:123:TYR:CZ     | 5:k:124:LYS:HG3    | 2.54                     | 0.41              |
| 6:l:284:ASN:HB3    | 6:l:290:LEU:HD11   | 2.02                     | 0.41              |
| 12:r:86:HIS:HB3    | 12:r:139:ARG:HG3   | 2.02                     | 0.41              |
| 17:w:17:LEU:HD11   | 17:w:81:LEU:HA     | 2.02                     | 0.41              |
| 21:0:23:LYS:HD3    | 21:0:23:LYS:HA     | 1.91                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:0:119:ARG:HE   | 21:0:119:ARG:HB2   | 1.59                     | 0.41              |
| 27:9:71:ASN:ND2   | 27:9:83:ASP:HA     | 2.36                     | 0.41              |
| 35:AH:9:ARG:HD2   | 35:AH:34:HIS:CE1   | 2.55                     | 0.41              |
| 46:B:544:U:H2'    | 46:B:545:U:C6      | 2.56                     | 0.41              |
| 46:B:824:U:H2'    | 46:B:825:U:C6      | 2.55                     | 0.41              |
| 46:B:1171:U:H2'   | 46:B:1172:U:O4'    | 2.20                     | 0.41              |
| 46:B:1236:U:O2'   | 46:B:1237:C:H5''   | 2.21                     | 0.41              |
| 46:B:1311:A:H2'   | 46:B:1312:C:H6     | 1.86                     | 0.41              |
| 46:B:1469:A:H2    | 46:B:1594:G:H1'    | 1.84                     | 0.41              |
| 48:D:61:LEU:HD21  | 48:D:96:LEU:HD21   | 2.02                     | 0.41              |
| 68:X:65:ALA:O     | 68:X:69:LEU:HD23   | 2.20                     | 0.41              |
| 77:g:13:LYS:O     | 77:g:17:GLN:HG2    | 2.20                     | 0.41              |
| 1:AS:121:A:N1     | 1:AS:144:G:O2'     | 2.47                     | 0.41              |
| 1:AS:602:A:H2'    | 1:AS:603:C:H6      | 1.85                     | 0.41              |
| 1:AS:1065:C:H2'   | 1:AS:1066:U:C6     | 2.55                     | 0.41              |
| 1:AS:1141:G:O6    | 1:AS:1154:A:H2     | 2.03                     | 0.41              |
| 1:AS:1193:A:N6    | 2:AT:86:U:C4       | 2.89                     | 0.41              |
| 1:AS:1341:U:H2'   | 1:AS:1342:G:O4'    | 2.20                     | 0.41              |
| 1:AS:1444:U:OP1   | 18:BK:67:ILE:HG22  | 2.20                     | 0.41              |
| 1:AS:2199:G:N2    | 1:AS:2202:A:OP2    | 2.30                     | 0.41              |
| 1:AS:2546:U:H5'   | 1:AS:2547:G:O4'    | 2.21                     | 0.41              |
| 1:AS:2558:G:C5    | 10:BC:242:LYS:HD2  | 2.55                     | 0.41              |
| 1:AS:2623:G:H5''  | 1:AS:2624:U:O4'    | 2.21                     | 0.41              |
| 1:AS:2625:C:O2'   | 1:AS:2629:A:N1     | 2.44                     | 0.41              |
| 1:AS:3275:A:OP1   | 18:BK:74:LYS:NZ    | 2.49                     | 0.41              |
| 3:AU:63:G:H1      | 3:AU:97:A:N6       | 2.18                     | 0.41              |
| 3:AU:104:A:OP2    | 3:AU:105:A:H5''    | 2.21                     | 0.41              |
| 3:AU:122:U:H2'    | 3:AU:123:G:H8      | 1.85                     | 0.41              |
| 4:AW:224:THR:HG22 | 4:AW:240:ALA:HB3   | 2.03                     | 0.41              |
| 5:AX:312:VAL:O    | 5:AX:332:LYS:HD3   | 2.21                     | 0.41              |
| 13:BF:109:HIS:CD2 | 13:BF:123:TYR:H    | 2.30                     | 0.41              |
| 28:BU:48:ARG:HD2  | 28:BU:69:LYS:HD2   | 2.02                     | 0.41              |
| 32:BY:109:GLU:O   | 32:BY:110:ASP:HB2  | 2.21                     | 0.41              |
| 44:CK:36:LYS:HB2  | 44:CK:45:ARG:NH1   | 2.34                     | 0.41              |
| 45:CL:107:TRP:CE3 | 50:CQ:143:LEU:HD12 | 2.55                     | 0.41              |
| 45:CL:120:GLU:CB  | 50:CQ:118:ARG:HG3  | 2.49                     | 0.41              |
| 46:CM:86:A:H1'    | 46:CM:146:A:H1'    | 2.02                     | 0.41              |
| 46:CM:246:U:C4'   | 58:CY:36:LYS:HD3   | 2.51                     | 0.41              |
| 46:CM:1051:C:H2'  | 46:CM:1052:G:H8    | 1.85                     | 0.41              |
| 48:CO:53:GLY:C    | 48:CO:55:LYS:H     | 2.28                     | 0.41              |
| 52:CS:30:PRO:O    | 52:CS:34:GLN:HG3   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:CZ:40:GLY:O    | 59:CZ:41:LEU:HD23 | 2.20                     | 0.41              |
| 61:DB:15:PHE:HB3  | 61:DB:22:PHE:HB2  | 2.00                     | 0.41              |
| 64:DE:11:ARG:HE   | 64:DE:11:ARG:HB3  | 1.45                     | 0.41              |
| 79:DT:74:ILE:HD12 | 79:DT:74:ILE:N    | 2.35                     | 0.41              |
| 79:DT:159:PRO:O   | 79:DT:161:ASP:N   | 2.50                     | 0.41              |
| 79:DT:293:ALA:C   | 79:DT:295:GLY:H   | 2.28                     | 0.41              |
| 81:P0:10:GLN:O    | 81:P0:13:SER:HB3  | 2.21                     | 0.41              |
| 81:P0:64:ARG:O    | 81:P0:67:LEU:HD23 | 2.20                     | 0.41              |
| 82:12:116:MET:C   | 82:12:118:HIS:H   | 2.29                     | 0.41              |
| 1:1:821:U:H5''    | 1:1:1793:A:C5     | 2.56                     | 0.41              |
| 1:1:1198:A:C2     | 1:1:2829:C:H5'    | 2.56                     | 0.41              |
| 1:1:1389:A:H5''   | 33:AF:100:SER:HB2 | 2.03                     | 0.41              |
| 1:1:1741:C:H2'    | 1:1:1742:U:H6     | 1.86                     | 0.41              |
| 1:1:1883:A:H4'    | 5:k:227:GLU:HA    | 2.03                     | 0.41              |
| 1:1:2330:A:H2'    | 1:1:2331:G:C8     | 2.56                     | 0.41              |
| 1:1:2632:G:O3'    | 1:1:2721:G:N2     | 2.54                     | 0.41              |
| 1:1:3300:A:H2'    | 1:1:3301:A:H8     | 1.84                     | 0.41              |
| 3:4:84:C:O3'      | 27:9:113:LYS:NZ   | 2.53                     | 0.41              |
| 6:l:331:TYR:HA    | 9:o:43:PHE:CE2    | 2.55                     | 0.41              |
| 20:z:162:ARG:O    | 20:z:165:ARG:HB3  | 2.20                     | 0.41              |
| 21:0:90:MET:HE3   | 21:0:90:MET:HB2   | 1.85                     | 0.41              |
| 34:AG:90:PRO:O    | 34:AG:93:THR:OG1  | 2.31                     | 0.41              |
| 46:B:267:G:H2'    | 46:B:268:C:C6     | 2.56                     | 0.41              |
| 46:B:526:U:C2     | 46:B:527:A:C8     | 3.08                     | 0.41              |
| 46:B:803:G:C4     | 46:B:838:G:N2     | 2.89                     | 0.41              |
| 62:R:75:VAL:HA    | 62:R:93:VAL:O     | 2.20                     | 0.41              |
| 65:U:129:TRP:HE3  | 65:U:131:LEU:HD12 | 1.86                     | 0.41              |
| 67:W:34:GLU:HG2   | 67:W:88:ARG:HH22  | 1.85                     | 0.41              |
| 1:AS:186:A:H2'    | 1:AS:187:U:C6     | 2.56                     | 0.41              |
| 1:AS:196:G:N2     | 1:AS:372:A:C8     | 2.88                     | 0.41              |
| 1:AS:290:G:H2'    | 1:AS:291:C:C6     | 2.55                     | 0.41              |
| 1:AS:321:C:H4'    | 16:BI:150:TRP:CG  | 2.56                     | 0.41              |
| 1:AS:656:G:H21    | 6:AY:94:MET:HB2   | 1.85                     | 0.41              |
| 1:AS:1562:G:OP1   | 1:AS:1562:G:O4'   | 2.39                     | 0.41              |
| 1:AS:1595:G:N2    | 1:AS:1605:C:C2    | 2.89                     | 0.41              |
| 1:AS:2430:G:P     | 1:AS:2430:G:O4'   | 2.78                     | 0.41              |
| 1:AS:2679:U:H2'   | 1:AS:2680:C:C6    | 2.56                     | 0.41              |
| 1:AS:2908:A:H2'   | 1:AS:2909:G:C8    | 2.56                     | 0.41              |
| 1:AS:2972:A:H2'   | 1:AS:2973:U:H6    | 1.86                     | 0.41              |
| 1:AS:3132:U:H2'   | 1:AS:3133:G:H8    | 1.85                     | 0.41              |
| 3:AU:83:U:H4'     | 3:AU:85:G:N3      | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AU:152:G:H2'     | 3:AU:153:U:O4'     | 2.21                     | 0.41              |
| 5:AX:92:TYR:HB2    | 5:AX:157:VAL:HB    | 2.01                     | 0.41              |
| 5:AX:284:ARG:NH1   | 5:AX:356:LEU:HD12  | 2.36                     | 0.41              |
| 80:BE:194:GLY:C    | 80:BE:196:TYR:H    | 2.27                     | 0.41              |
| 13:BF:92:ARG:HG2   | 13:BF:93:SER:N     | 2.36                     | 0.41              |
| 27:BT:77:LYS:HE3   | 40:CG:31:THR:HG21  | 2.02                     | 0.41              |
| 28:BU:17:ARG:HD3   | 35:CB:73:GLN:HB3   | 2.02                     | 0.41              |
| 31:BX:12:ILE:HD12  | 31:BX:12:ILE:H     | 1.85                     | 0.41              |
| 39:CF:25:VAL:O     | 39:CF:78:LEU:N     | 2.46                     | 0.41              |
| 46:CM:159:U:O2'    | 46:CM:160:A:H5'    | 2.21                     | 0.41              |
| 46:CM:258:U:H5     | 55:CV:43:ILE:O     | 2.04                     | 0.41              |
| 46:CM:260:U:C2'    | 46:CM:261:C:H5'    | 2.51                     | 0.41              |
| 46:CM:835:A:H2'    | 46:CM:836:U:C6     | 2.55                     | 0.41              |
| 46:CM:867:U:H2'    | 46:CM:868:C:C6     | 2.56                     | 0.41              |
| 46:CM:1239:U:H2'   | 46:CM:1240:G:O4'   | 2.21                     | 0.41              |
| 46:CM:1460:G:C2    | 46:CM:1461:A:C5    | 3.09                     | 0.41              |
| 48:CO:152:LYS:HD2  | 48:CO:152:LYS:HA   | 1.84                     | 0.41              |
| 48:CO:166:LYS:HE2  | 48:CO:166:LYS:HB3  | 1.80                     | 0.41              |
| 53:CT:161:GLU:HB3  | 53:CT:170:THR:HG22 | 2.02                     | 0.41              |
| 54:CU:66:TYR:O     | 54:CU:70:GLN:N     | 2.54                     | 0.41              |
| 62:DC:121:ILE:HG22 | 62:DC:123:TYR:H    | 1.86                     | 0.41              |
| 77:DR:32:GLY:O     | 77:DR:33:ARG:C     | 2.64                     | 0.41              |
| 79:DT:156:ARG:HB3  | 79:DT:201:LEU:HD22 | 2.02                     | 0.41              |
| 79:DT:158:SER:C    | 79:DT:160:SER:H    | 2.28                     | 0.41              |
| 79:DT:172:ASP:OD1  | 79:DT:172:ASP:N    | 2.54                     | 0.41              |
| 79:DT:259:ILE:HD11 | 79:DT:271:LEU:HD21 | 2.03                     | 0.41              |
| 1:1:38:A:H5''      | 29:AB:35:ALA:HB2   | 2.02                     | 0.41              |
| 1:1:239:A:H3'      | 1:1:240:C:O4'      | 2.21                     | 0.41              |
| 1:1:292:U:OP1      | 1:1:2410:A:H1'     | 2.20                     | 0.41              |
| 1:1:342:A:C4       | 1:1:368:G:N7       | 2.89                     | 0.41              |
| 1:1:359:U:H4'      | 1:1:813:A:H62      | 1.86                     | 0.41              |
| 1:1:531:G:N2       | 1:1:552:G:O2'      | 2.49                     | 0.41              |
| 1:1:574:C:OP1      | 9:o:238:LYS:NZ     | 2.32                     | 0.41              |
| 1:1:707:A:H1'      | 1:1:2759:G:O2'     | 2.20                     | 0.41              |
| 1:1:1022:A:C2      | 1:1:1023:A:H1'     | 2.55                     | 0.41              |
| 1:1:1222:G:H2'     | 1:1:1223:C:C6      | 2.56                     | 0.41              |
| 1:1:1365:A:H4'     | 29:AB:21:ARG:HG3   | 2.03                     | 0.41              |
| 1:1:1533:A:H2'     | 1:1:1534:G:O4'     | 2.21                     | 0.41              |
| 1:1:1630:G:C6      | 1:1:1636:G:C6      | 3.09                     | 0.41              |
| 1:1:1656:C:H2'     | 1:1:1657:G:C8      | 2.56                     | 0.41              |
| 1:1:1767:G:H2'     | 1:1:1768:U:O4'     | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:2129:C:O2'    | 1:1:2221:A:N1     | 2.47                     | 0.41              |
| 1:1:2156:A:H5''   | 4:j:129:THR:OG1   | 2.21                     | 0.41              |
| 1:1:2174:C:OP1    | 46:B:980:A:H4'    | 2.21                     | 0.41              |
| 1:1:2262:C:C4     | 1:1:2286:C:O4'    | 2.74                     | 0.41              |
| 1:1:2367:C:H2'    | 1:1:2368:A:H8     | 1.85                     | 0.41              |
| 1:1:2445:G:O2'    | 1:1:2446:A:O4'    | 2.39                     | 0.41              |
| 1:1:2457:C:H5'    | 1:1:2458:G:OP2    | 2.21                     | 0.41              |
| 1:1:2485:U:H6     | 1:1:2485:U:O5'    | 2.04                     | 0.41              |
| 1:1:2649:G:H2'    | 1:1:2649:G:N3     | 2.34                     | 0.41              |
| 1:1:2695:U:H2'    | 1:1:2696:U:C6     | 2.56                     | 0.41              |
| 1:1:2737:C:O3'    | 43:AP:39:GLY:HA3  | 2.21                     | 0.41              |
| 1:1:2830:U:H2'    | 1:1:2831:U:C6     | 2.56                     | 0.41              |
| 1:1:2981:G:OP1    | 17:w:67:LYS:HD2   | 2.21                     | 0.41              |
| 1:1:3197:G:H2'    | 1:1:3198:C:H6     | 1.84                     | 0.41              |
| 1:1:3201:U:H1'    | 1:1:3217:G:N2     | 2.36                     | 0.41              |
| 2:3:59:U:H2'      | 2:3:60:G:H8       | 1.86                     | 0.41              |
| 2:3:100:C:OP2     | 21:0:52:LYS:HE3   | 2.21                     | 0.41              |
| 3:4:6:U:H2'       | 3:4:7:U:C6        | 2.56                     | 0.41              |
| 3:4:67:U:H5''     | 38:AK:85:ALA:HB2  | 2.01                     | 0.41              |
| 3:4:143:U:H2'     | 3:4:144:G:O4'     | 2.20                     | 0.41              |
| 5:k:133:TYR:O     | 5:k:136:LYS:HB2   | 2.21                     | 0.41              |
| 9:o:14:GLU:CD     | 9:o:14:GLU:H      | 2.29                     | 0.41              |
| 10:p:144:ILE:HG21 | 10:p:170:LEU:HG   | 2.02                     | 0.41              |
| 11:q:47:LYS:HE3   | 15:u:3:SER:HB2    | 2.03                     | 0.41              |
| 11:q:85:GLY:HA3   | 11:q:187:ILE:HD12 | 2.03                     | 0.41              |
| 12:r:42:THR:OG1   | 12:r:45:GLU:HG3   | 2.20                     | 0.41              |
| 16:v:43:SER:OG    | 16:v:131:GLU:OE2  | 2.23                     | 0.41              |
| 18:x:60:PHE:HB3   | 18:x:64:ASN:HB3   | 2.03                     | 0.41              |
| 19:y:104:LEU:HA   | 19:y:104:LEU:HD23 | 1.83                     | 0.41              |
| 21:0:109:ASP:OD2  | 21:0:113:ARG:NH1  | 2.54                     | 0.41              |
| 29:AB:63:LYS:HE2  | 29:AB:65:GLN:NE2  | 2.36                     | 0.41              |
| 31:AD:11:ASN:O    | 31:AD:14:SER:N    | 2.43                     | 0.41              |
| 46:B:378:U:C4     | 56:L:5:PRO:HB3    | 2.56                     | 0.41              |
| 46:B:475:A:H5'    | 77:g:34:ALA:CB    | 2.51                     | 0.41              |
| 46:B:484:G:H2'    | 46:B:485:G:C8     | 2.56                     | 0.41              |
| 46:B:584:G:C6     | 46:B:585:C:C4     | 3.09                     | 0.41              |
| 46:B:734:U:H2'    | 46:B:735:U:C6     | 2.55                     | 0.41              |
| 46:B:862:G:H22    | 46:B:936:A:H2     | 1.67                     | 0.41              |
| 46:B:931:U:H4'    | 48:D:165:ARG:HD3  | 2.02                     | 0.41              |
| 46:B:1215:A:H2    | 46:B:1243:U:O2    | 2.04                     | 0.41              |
| 46:B:1239:U:H2'   | 46:B:1240:G:C8    | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:1334:G:H2'   | 46:B:1335:U:C6    | 2.56                     | 0.41              |
| 51:G:199:GLU:OE2  | 51:G:207:LEU:HD12 | 2.21                     | 0.41              |
| 52:H:97:LEU:HD23  | 52:H:97:LEU:HA    | 1.92                     | 0.41              |
| 56:L:126:ARG:HD2  | 77:g:33:ARG:HD3   | 2.01                     | 0.41              |
| 57:M:56:LYS:NZ    | 57:M:69:THR:HG22  | 2.35                     | 0.41              |
| 59:O:67:THR:C     | 59:O:69:GLU:H     | 2.29                     | 0.41              |
| 60:P:87:ASP:N     | 60:P:87:ASP:OD1   | 2.53                     | 0.41              |
| 62:R:121:ILE:HG23 | 62:R:123:TYR:C    | 2.46                     | 0.41              |
| 63:S:38:VAL:HG13  | 63:S:40:PRO:HD2   | 2.02                     | 0.41              |
| 63:S:46:LYS:HD2   | 63:S:46:LYS:HA    | 1.72                     | 0.41              |
| 64:T:16:LEU:HD23  | 64:T:16:LEU:HA    | 1.86                     | 0.41              |
| 66:V:64:HIS:CE1   | 66:V:68:ARG:HE    | 2.39                     | 0.41              |
| 66:V:108:LEU:HD23 | 66:V:114:LEU:HD23 | 2.02                     | 0.41              |
| 69:Y:81:VAL:HG21  | 69:Y:125:ILE:HB   | 2.02                     | 0.41              |
| 72:b:66:VAL:HG22  | 72:b:71:ILE:O     | 2.21                     | 0.41              |
| 75:e:18:ARG:HD2   | 75:e:26:THR:HG22  | 2.03                     | 0.41              |
| 76:f:24:CYS:SG    | 76:f:26:SER:HB2   | 2.60                     | 0.41              |
| 78:h:160:ARG:HH11 | 78:h:160:ARG:HA   | 1.86                     | 0.41              |
| 1:AS:284:A:C5     | 1:AS:306:A:H1'    | 2.55                     | 0.41              |
| 1:AS:440:U:O2'    | 1:AS:441:U:H3'    | 2.20                     | 0.41              |
| 1:AS:635:C:C2     | 1:AS:636:C:C5     | 3.09                     | 0.41              |
| 1:AS:780:A:O2'    | 1:AS:781:G:OP2    | 2.36                     | 0.41              |
| 1:AS:851:U:C4     | 1:AS:852:G:C6     | 3.08                     | 0.41              |
| 1:AS:962:U:H2'    | 1:AS:963:A:H8     | 1.84                     | 0.41              |
| 1:AS:987:G:C6     | 1:AS:1055:G:C5    | 3.09                     | 0.41              |
| 1:AS:1134:U:O3'   | 9:BB:95:PRO:HD3   | 2.21                     | 0.41              |
| 1:AS:1227:A:H8    | 1:AS:1227:A:O5'   | 2.03                     | 0.41              |
| 1:AS:1302:G:C6    | 17:BJ:63:THR:HA   | 2.56                     | 0.41              |
| 1:AS:1506:G:H2'   | 1:AS:1508:U:C4    | 2.56                     | 0.41              |
| 1:AS:1559:C:O2'   | 1:AS:1560:U:OP1   | 2.29                     | 0.41              |
| 1:AS:1616:U:H2'   | 1:AS:1617:A:C8    | 2.56                     | 0.41              |
| 1:AS:2089:G:H5''  | 25:BR:48:ARG:CZ   | 2.51                     | 0.41              |
| 1:AS:2260:U:O2    | 1:AS:2288:U:H4'   | 2.21                     | 0.41              |
| 1:AS:2375:A:H2'   | 1:AS:2845:U:O4'   | 2.20                     | 0.41              |
| 1:AS:2481:G:H2'   | 1:AS:2482:U:H6    | 1.86                     | 0.41              |
| 1:AS:2649:G:O2'   | 1:AS:2651:A:N1    | 2.50                     | 0.41              |
| 1:AS:2936:G:O2'   | 1:AS:2938:G:N7    | 2.51                     | 0.41              |
| 2:AT:49:G:H4'     | 2:AT:50:U:C5'     | 2.51                     | 0.41              |
| 3:AU:3:A:O2'      | 18:BK:61:ARG:HD3  | 2.20                     | 0.41              |
| 3:AU:27:U:H2'     | 3:AU:28:C:H6      | 1.86                     | 0.41              |
| 4:AW:130:SER:HB2  | 4:AW:171:GLY:C    | 2.45                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AW:227:ARG:HB2   | 4:AW:239:ALA:HB2   | 2.03                     | 0.41              |
| 5:AX:133:TYR:O     | 5:AX:136:LYS:HB2   | 2.21                     | 0.41              |
| 7:AZ:96:SER:OG     | 7:AZ:198:TYR:O     | 2.39                     | 0.41              |
| 9:BB:158:ARG:HD2   | 9:BB:201:TRP:CD1   | 2.56                     | 0.41              |
| 10:BC:69:ARG:HA    | 10:BC:238:ILE:O    | 2.21                     | 0.41              |
| 10:BC:144:ILE:HG12 | 10:BC:152:VAL:HG21 | 2.02                     | 0.41              |
| 14:BG:62:THR:O     | 14:BG:66:ASN:OD1   | 2.39                     | 0.41              |
| 14:BG:134:GLU:HA   | 14:BG:137:SER:HB3  | 2.03                     | 0.41              |
| 16:BI:94:TYR:OH    | 16:BI:96:LYS:HE2   | 2.21                     | 0.41              |
| 16:BI:122:ASN:OD1  | 16:BI:123:GLN:N    | 2.47                     | 0.41              |
| 18:BK:21:TYR:CD1   | 18:BK:123:PRO:HD2  | 2.55                     | 0.41              |
| 22:BO:92:ARG:HB3   | 22:BO:94:GLU:OE1   | 2.21                     | 0.41              |
| 23:BP:20:ALA:O     | 23:BP:23:VAL:N     | 2.54                     | 0.41              |
| 23:BP:59:GLU:OE1   | 23:BP:60:SER:N     | 2.50                     | 0.41              |
| 25:BR:2:LYS:HE2    | 25:BR:4:GLU:OE2    | 2.20                     | 0.41              |
| 25:BR:89:LEU:HD23  | 25:BR:90:ILE:HD13  | 2.03                     | 0.41              |
| 25:BR:111:LYS:HD3  | 46:CM:278:U:H3     | 1.86                     | 0.41              |
| 26:BS:64:VAL:O     | 36:CC:32:LYS:NZ    | 2.29                     | 0.41              |
| 26:BS:73:MET:O     | 26:BS:77:GLU:HG2   | 2.20                     | 0.41              |
| 33:BZ:33:TRP:CH2   | 33:BZ:53:GLN:HG2   | 2.56                     | 0.41              |
| 34:CA:20:LYS:HE2   | 34:CA:20:LYS:HB2   | 1.72                     | 0.41              |
| 35:CB:105:LEU:O    | 35:CB:106:LYS:C    | 2.64                     | 0.41              |
| 36:CC:5:LYS:HA     | 36:CC:5:LYS:HD3    | 1.95                     | 0.41              |
| 36:CC:85:THR:HG22  | 36:CC:88:LEU:HB2   | 2.02                     | 0.41              |
| 43:CJ:65:THR:OG1   | 43:CJ:87:ARG:HB3   | 2.21                     | 0.41              |
| 46:CM:221:U:C2     | 46:CM:823:G:C2     | 3.09                     | 0.41              |
| 46:CM:224:A:C2     | 46:CM:820:U:N3     | 2.89                     | 0.41              |
| 46:CM:310:A:C2     | 46:CM:312:C:H2'    | 2.56                     | 0.41              |
| 46:CM:472:A:N1     | 46:CM:592:A:H5'    | 2.35                     | 0.41              |
| 46:CM:701:G:H5'    | 53:CT:230:ARG:HH12 | 1.86                     | 0.41              |
| 46:CM:732:C:H2'    | 46:CM:733:U:C6     | 2.56                     | 0.41              |
| 46:CM:824:U:C4     | 46:CM:825:U:C5     | 3.09                     | 0.41              |
| 46:CM:852:G:H21    | 60:DA:87:ASP:CG    | 2.28                     | 0.41              |
| 46:CM:1131:G:O2'   | 46:CM:1622:A:N1    | 2.49                     | 0.41              |
| 46:CM:1286:U:H5'   | 49:CP:83:LYS:CD    | 2.51                     | 0.41              |
| 46:CM:1595:U:O3'   | 63:DD:72:GLY:HA3   | 2.20                     | 0.41              |
| 46:CM:1771:C:H2'   | 46:CM:1772:U:C6    | 2.56                     | 0.41              |
| 48:CO:56:ASN:O     | 48:CO:58:ALA:N     | 2.54                     | 0.41              |
| 48:CO:181:LEU:O    | 48:CO:185:THR:HG23 | 2.21                     | 0.41              |
| 49:CP:138:TYR:OH   | 49:CP:144:GLY:O    | 2.21                     | 0.41              |
| 50:CQ:48:GLU:HG2   | 50:CQ:88:TYR:CE2   | 2.41                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:CQ:110:LEU:HD21 | 50:CQ:116:ILE:HG22 | 2.03                     | 0.41              |
| 50:CQ:140:SER:O    | 50:CQ:184:GLY:N    | 2.53                     | 0.41              |
| 51:CR:22:LYS:HB3   | 56:CW:4:ALA:HB3    | 2.02                     | 0.41              |
| 54:CU:40:LYS:HE3   | 54:CU:60:PRO:HD3   | 2.03                     | 0.41              |
| 57:CX:28:ASN:HD21  | 76:DQ:7:TRP:NE1    | 2.19                     | 0.41              |
| 59:CZ:113:ARG:O    | 59:CZ:115:VAL:HG13 | 2.21                     | 0.41              |
| 62:DC:11:THR:OG1   | 62:DC:12:PHE:N     | 2.50                     | 0.41              |
| 62:DC:97:TYR:HB2   | 62:DC:102:PHE:CE1  | 2.56                     | 0.41              |
| 64:DE:99:GLN:HG2   | 64:DE:118:PRO:HB2  | 2.03                     | 0.41              |
| 71:DL:34:ASN:OD1   | 71:DL:34:ASN:N     | 2.53                     | 0.41              |
| 72:DM:54:VAL:HG13  | 72:DM:60:VAL:HG11  | 2.02                     | 0.41              |
| 79:DT:5:GLU:CD     | 79:DT:312:VAL:HB   | 2.46                     | 0.41              |
| 79:DT:18:GLY:C     | 79:DT:305:ASN:OD1  | 2.64                     | 0.41              |
| 79:DT:21:THR:HG23  | 79:DT:38:ARG:N     | 2.36                     | 0.41              |
| 79:DT:44:LYS:NZ    | 79:DT:95:LEU:HD12  | 2.36                     | 0.41              |
| 79:DT:156:ARG:HB2  | 79:DT:167:ILE:HD12 | 2.03                     | 0.41              |
| 79:DT:156:ARG:HB2  | 79:DT:167:ILE:CD1  | 2.51                     | 0.41              |
| 79:DT:199:ILE:HD13 | 79:DT:199:ILE:HA   | 1.82                     | 0.41              |
| 79:DT:221:ASP:CB   | 79:DT:226:LYS:HB3  | 2.49                     | 0.41              |
| 81:P0:11:TYR:O     | 81:P0:15:LEU:HB2   | 2.20                     | 0.41              |
| 82:12:110:PHE:O    | 82:12:113:ALA:HB3  | 2.21                     | 0.41              |
| 1:1:618:U:H2'      | 18:x:167:ARG:HH11  | 1.84                     | 0.41              |
| 1:1:669:U:O2'      | 19:y:20:LYS:HG2    | 2.21                     | 0.41              |
| 1:1:976:A:C2'      | 1:1:977:U:H5'      | 2.50                     | 0.41              |
| 1:1:985:A:H2'      | 1:1:986:U:O4'      | 2.21                     | 0.41              |
| 1:1:1096:U:OP1     | 9:o:116:ARG:NH2    | 2.45                     | 0.41              |
| 1:1:1494:A:H2'     | 1:1:1495:U:C6      | 2.56                     | 0.41              |
| 1:1:1556:G:C2      | 1:1:1575:A:C8      | 3.09                     | 0.41              |
| 1:1:1695:A:C6      | 1:1:1743:G:C6      | 3.09                     | 0.41              |
| 1:1:1907:A:H2      | 1:1:2100:G:C8      | 2.39                     | 0.41              |
| 1:1:2191:A:N1      | 1:1:2407:G:H1'     | 2.35                     | 0.41              |
| 1:1:2498:A:H2'     | 1:1:2499:U:C6      | 2.56                     | 0.41              |
| 1:1:3234:U:H4'     | 1:1:3235:A:O5'     | 2.20                     | 0.41              |
| 3:4:83:U:H4'       | 3:4:85:G:N3        | 2.36                     | 0.41              |
| 5:k:369:ARG:HD2    | 25:7:11:SER:HB3    | 2.03                     | 0.41              |
| 6:l:25:ALA:HB3     | 6:l:265:SER:HA     | 2.02                     | 0.41              |
| 11:q:77:ASN:HA     | 11:q:80:THR:HG22   | 2.03                     | 0.41              |
| 15:u:34:ASP:OD2    | 15:u:37:ARG:NH2    | 2.54                     | 0.41              |
| 15:u:106:SER:O     | 15:u:110:ARG:HG3   | 2.21                     | 0.41              |
| 18:x:180:LYS:HE2   | 18:x:180:LYS:HB3   | 1.50                     | 0.41              |
| 26:8:89:LYS:H      | 26:8:89:LYS:HG3    | 1.69                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:B:20:G:H5'     | 46:B:569:G:C8     | 2.56                     | 0.41              |
| 46:B:55:A:N6      | 46:B:401:G:H1'    | 2.36                     | 0.41              |
| 46:B:398:A:H5''   | 55:K:24:LYS:O     | 2.21                     | 0.41              |
| 46:B:485:G:N2     | 46:B:499:U:C2     | 2.89                     | 0.41              |
| 46:B:517:C:H6     | 46:B:517:C:H2'    | 1.66                     | 0.41              |
| 46:B:551:G:N2     | 46:B:569:G:N7     | 2.69                     | 0.41              |
| 46:B:670:C:H6     | 46:B:670:C:H2'    | 1.64                     | 0.41              |
| 46:B:1276:G:H1    | 46:B:1309:G:N2    | 2.09                     | 0.41              |
| 46:B:1469:A:C2    | 46:B:1594:G:H1'   | 2.56                     | 0.41              |
| 46:B:1670:U:HO2'  | 46:B:1671:G:P     | 2.41                     | 0.41              |
| 47:C:163:ASN:OD1  | 47:C:166:GLY:N    | 2.54                     | 0.41              |
| 47:C:171:GLY:HA3  | 47:C:203:PHE:CE1  | 2.55                     | 0.41              |
| 49:E:168:PRO:HG3  | 56:L:57:ARG:HG3   | 2.03                     | 0.41              |
| 55:K:76:THR:HG21  | 55:K:104:ILE:HD12 | 2.02                     | 0.41              |
| 55:K:159:GLU:HB3  | 55:K:162:VAL:HG23 | 2.03                     | 0.41              |
| 57:M:27:PHE:N     | 57:M:27:PHE:CD1   | 2.89                     | 0.41              |
| 65:U:129:TRP:HE3  | 65:U:131:LEU:CD1  | 2.34                     | 0.41              |
| 79:AR:34:LEU:HG   | 79:AR:72:VAL:HG11 | 2.03                     | 0.41              |
| 79:AR:46:LYS:O    | 79:AR:56:GLY:HA2  | 2.21                     | 0.41              |
| 79:AR:162:GLN:C   | 79:AR:164:SER:H   | 2.29                     | 0.41              |
| 79:AR:252:ALA:HB1 | 79:AR:286:ALA:O   | 2.21                     | 0.41              |
| 1:AS:424:G:O2'    | 33:BZ:24:ASP:OD2  | 2.26                     | 0.41              |
| 1:AS:629:A:H2'    | 1:AS:630:G:H8     | 1.86                     | 0.41              |
| 1:AS:975:U:H4'    | 1:AS:976:A:O5'    | 2.21                     | 0.41              |
| 1:AS:1610:C:H2'   | 1:AS:1611:U:C6    | 2.56                     | 0.41              |
| 1:AS:2356:C:H2'   | 1:AS:2357:U:H6    | 1.86                     | 0.41              |
| 1:AS:2608:A:H5''  | 1:AS:2609:A:H5'   | 2.03                     | 0.41              |
| 1:AS:2981:G:H5''  | 17:BJ:67:LYS:HG3  | 2.02                     | 0.41              |
| 1:AS:3024:G:H2'   | 1:AS:3025:G:H8    | 1.86                     | 0.41              |
| 1:AS:3232:G:H2'   | 8:BA:68:PHE:CZ    | 2.56                     | 0.41              |
| 2:AT:24:A:H2'     | 2:AT:25:G:O4'     | 2.21                     | 0.41              |
| 7:AZ:41:LYS:HD3   | 7:AZ:41:LYS:HA    | 1.92                     | 0.41              |
| 13:BF:63:GLU:O    | 13:BF:65:ILE:HG12 | 2.21                     | 0.41              |
| 21:BN:115:ARG:O   | 21:BN:117:ARG:NH1 | 2.53                     | 0.41              |
| 28:BU:34:LYS:C    | 28:BU:36:HIS:N    | 2.78                     | 0.41              |
| 36:CC:4:VAL:CG1   | 36:CC:53:ARG:HD2  | 2.51                     | 0.41              |
| 38:CE:82:VAL:HG12 | 38:CE:83:ALA:N    | 2.35                     | 0.41              |
| 40:CG:30:ARG:HB2  | 40:CG:33:ASN:HB2  | 2.03                     | 0.41              |
| 46:CM:138:C:H5''  | 46:CM:139:U:C6    | 2.56                     | 0.41              |
| 46:CM:189:G:N7    | 55:CV:143:ARG:NH2 | 2.68                     | 0.41              |
| 46:CM:233:G:H8    | 46:CM:233:G:OP2   | 2.04                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CM:327:G:H2'    | 46:CM:328:G:H8     | 1.86                     | 0.41              |
| 46:CM:402:G:H2'    | 46:CM:403:C:H6     | 1.86                     | 0.41              |
| 46:CM:1315:G:C2    | 46:CM:1316:A:H1'   | 2.55                     | 0.41              |
| 52:CS:55:ASP:C     | 52:CS:57:SER:H     | 2.28                     | 0.41              |
| 53:CT:64:LYS:HB2   | 53:CT:97:VAL:HG21  | 2.03                     | 0.41              |
| 53:CT:127:THR:OG1  | 53:CT:128:THR:N    | 2.54                     | 0.41              |
| 54:CU:120:LYS:HD3  | 54:CU:120:LYS:HA   | 1.82                     | 0.41              |
| 57:CX:25:LYS:HD2   | 57:CX:59:PHE:CZ    | 2.55                     | 0.41              |
| 59:CZ:35:SER:HA    | 59:CZ:127:GLY:HA3  | 2.02                     | 0.41              |
| 62:DC:125:PRO:CG   | 62:DC:127:ARG:HH12 | 2.34                     | 0.41              |
| 78:DS:161:ARG:NH2  | 78:DS:163:CYS:C    | 2.79                     | 0.41              |
| 78:DS:165:ALA:C    | 78:DS:167:THR:N    | 2.79                     | 0.41              |
| 81:P0:2:GLY:O      | 81:P0:4:ALA:N      | 2.54                     | 0.41              |
| 81:P0:73:PHE:C     | 81:P0:75:LYS:N     | 2.79                     | 0.41              |
| 81:P0:104:VAL:HG12 | 81:P0:106:ALA:H    | 1.86                     | 0.41              |
| 1:1:109:G:OP2      | 14:t:73:ARG:NH2    | 2.53                     | 0.40              |
| 1:1:515:A:C6       | 1:1:518:A:H4'      | 2.56                     | 0.40              |
| 1:1:630:G:H2'      | 1:1:631:U:C6       | 2.57                     | 0.40              |
| 1:1:1249:U:OP2     | 1:1:1249:U:H2'     | 2.21                     | 0.40              |
| 1:1:1251:C:O2'     | 1:1:1252:G:H5'     | 2.20                     | 0.40              |
| 1:1:2433:U:C2      | 1:1:2434:A:C8      | 3.09                     | 0.40              |
| 1:1:2656:C:H2'     | 1:1:2657:C:H6      | 1.87                     | 0.40              |
| 1:1:3202:U:H2'     | 1:1:3203:A:C8      | 2.56                     | 0.40              |
| 1:1:3232:G:H2'     | 8:n:68:PHE:CZ      | 2.56                     | 0.40              |
| 3:4:13:A:O2'       | 18:x:120:ASN:HB3   | 2.21                     | 0.40              |
| 3:4:68:A:H2'       | 3:4:69:U:C6        | 2.57                     | 0.40              |
| 4:j:180:LEU:HD21   | 44:AQ:22:LEU:HB3   | 2.02                     | 0.40              |
| 5:k:67:MET:SD      | 5:k:70:ARG:HD2     | 2.61                     | 0.40              |
| 10:p:83:LEU:HD23   | 10:p:83:LEU:HA     | 1.78                     | 0.40              |
| 19:y:44:PHE:CD2    | 19:y:134:GLY:HA3   | 2.56                     | 0.40              |
| 19:y:170:ARG:HA    | 19:y:174:ARG:HD2   | 2.02                     | 0.40              |
| 32:AE:84:ALA:C     | 32:AE:86:GLU:H     | 2.28                     | 0.40              |
| 35:AH:83:ASN:O     | 35:AH:87:GLU:HG3   | 2.21                     | 0.40              |
| 46:B:98:U:H2'      | 46:B:99:C:C6       | 2.56                     | 0.40              |
| 46:B:857:G:H22     | 46:B:1032:G:H4'    | 1.86                     | 0.40              |
| 46:B:1109:A:H2'    | 46:B:1110:A:C8     | 2.56                     | 0.40              |
| 46:B:1376:U:C5     | 64:T:3:ARG:HG3     | 2.56                     | 0.40              |
| 46:B:1512:A:H4'    | 66:V:83:ALA:HB2    | 2.03                     | 0.40              |
| 47:C:54:TRP:O      | 47:C:58:VAL:HG23   | 2.21                     | 0.40              |
| 50:F:77:ARG:HB2    | 57:M:22:VAL:HG11   | 2.01                     | 0.40              |
| 54:J:60:PRO:N      | 54:J:61:PRO:HD2    | 2.36                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:J:122:LEU:HB2  | 54:J:169:TYR:HE2   | 1.85                     | 0.40              |
| 60:P:5:HIS:CE1    | 60:P:121:ARG:HG3   | 2.56                     | 0.40              |
| 63:S:40:PRO:O     | 63:S:41:GLU:C      | 2.63                     | 0.40              |
| 64:T:77:GLU:O     | 64:T:81:LYS:HB2    | 2.21                     | 0.40              |
| 67:W:56:ARG:HA    | 67:W:88:ARG:HG3    | 2.03                     | 0.40              |
| 71:a:42:GLU:HG3   | 71:a:52:LYS:HE3    | 2.03                     | 0.40              |
| 74:d:73:LEU:HD11  | 74:d:79:PHE:HB3    | 2.04                     | 0.40              |
| 78:h:180:ARG:HB2  | 78:h:189:THR:HB    | 2.03                     | 0.40              |
| 79:AR:104:PHE:CE2 | 79:AR:139:GLY:HA2  | 2.56                     | 0.40              |
| 1:AS:50:A:C4      | 1:AS:51:A:C8       | 3.09                     | 0.40              |
| 1:AS:166:U:H2'    | 1:AS:167:U:H6      | 1.84                     | 0.40              |
| 1:AS:264:G:P      | 37:CD:34:GLN:HE22  | 2.44                     | 0.40              |
| 1:AS:304:G:H3'    | 1:AS:304:G:OP2     | 2.21                     | 0.40              |
| 1:AS:495:C:H2'    | 1:AS:496:A:H8      | 1.86                     | 0.40              |
| 1:AS:684:G:P      | 14:BG:39:ARG:HH21  | 2.44                     | 0.40              |
| 1:AS:1227:A:H5''  | 1:AS:1228:C:C5'    | 2.51                     | 0.40              |
| 3:AU:81:A:H2'     | 3:AU:82:U:C6       | 2.56                     | 0.40              |
| 6:AY:316:LYS:HD3  | 6:AY:321:ASN:ND2   | 2.36                     | 0.40              |
| 7:AZ:40:HIS:CE1   | 7:AZ:42:ALA:HB3    | 2.56                     | 0.40              |
| 8:BA:30:ARG:HD3   | 34:CA:106:ASN:HD22 | 1.85                     | 0.40              |
| 9:BB:124:LEU:HD23 | 9:BB:124:LEU:HA    | 1.83                     | 0.40              |
| 80:BE:19:LYS:HD2  | 80:BE:26:VAL:HB    | 2.03                     | 0.40              |
| 36:CC:59:ASN:O    | 36:CC:63:ARG:HB2   | 2.21                     | 0.40              |
| 45:CL:65:LYS:HD3  | 62:DC:105:VAL:CG1  | 2.51                     | 0.40              |
| 46:CM:481:A:N1    | 46:CM:503:A:C6     | 2.89                     | 0.40              |
| 46:CM:696:U:OP1   | 46:CM:696:U:C6     | 2.74                     | 0.40              |
| 46:CM:824:U:C5    | 46:CM:825:U:C5     | 3.09                     | 0.40              |
| 46:CM:853:G:C2    | 46:CM:946:U:C2     | 3.09                     | 0.40              |
| 46:CM:915:A:O2'   | 48:CO:111:ARG:NH2  | 2.54                     | 0.40              |
| 46:CM:1140:G:H2'  | 46:CM:1141:C:H6    | 1.84                     | 0.40              |
| 46:CM:1239:U:H2'  | 46:CM:1240:G:C8    | 2.56                     | 0.40              |
| 46:CM:1258:G:N2   | 46:CM:1263:G:O6    | 2.54                     | 0.40              |
| 46:CM:1459:U:O2'  | 52:CS:103:ASN:ND2  | 2.53                     | 0.40              |
| 48:CO:162:ARG:HG2 | 48:CO:165:ARG:NH2  | 2.26                     | 0.40              |
| 50:CQ:65:ARG:HD2  | 57:CX:91:ARG:NE    | 2.36                     | 0.40              |
| 53:CT:137:ARG:HD3 | 53:CT:177:ARG:HD2  | 2.02                     | 0.40              |
| 57:CX:55:VAL:HG12 | 57:CX:68:LEU:HA    | 2.03                     | 0.40              |
| 62:DC:64:ARG:HH12 | 62:DC:92:SER:H     | 1.69                     | 0.40              |
| 63:DD:23:ALA:HB2  | 63:DD:91:TYR:OH    | 2.22                     | 0.40              |
| 64:DE:36:SER:OG   | 64:DE:47:ARG:NH1   | 2.43                     | 0.40              |
| 70:DK:70:LYS:HB3  | 70:DK:93:LEU:HD22  | 2.02                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:DM:54:VAL:N     | 72:DM:55:PRO:HD2   | 2.36                     | 0.40              |
| 74:DO:49:HIS:HA    | 74:DO:70:LYS:HA    | 2.03                     | 0.40              |
| 79:DT:91:ARG:HD3   | 79:DT:100:THR:HG21 | 2.03                     | 0.40              |
| 79:DT:262:LEU:HD22 | 79:DT:263:GLN:H    | 1.82                     | 0.40              |
| 82:12:123:LYS:H    | 82:12:123:LYS:HG3  | 1.61                     | 0.40              |
| 1:1:138:G:H2'      | 1:1:139:U:C6       | 2.56                     | 0.40              |
| 1:1:196:G:C6       | 1:1:197:A:C6       | 3.10                     | 0.40              |
| 1:1:288:C:O2'      | 16:v:95:GLN:O      | 2.39                     | 0.40              |
| 1:1:781:G:N2       | 1:1:782:A:H62      | 2.19                     | 0.40              |
| 1:1:892:A:H5'      | 4:j:183:GLY:HA2    | 2.02                     | 0.40              |
| 1:1:997:G:H1'      | 1:1:1037:U:H5'     | 2.03                     | 0.40              |
| 1:1:1010:U:H2'     | 1:1:1011:C:H5''    | 2.04                     | 0.40              |
| 1:1:1900:C:H2'     | 1:1:1901:G:O4'     | 2.21                     | 0.40              |
| 1:1:2184:G:N1      | 1:1:2214:G:O6      | 2.54                     | 0.40              |
| 1:1:2545:C:O2'     | 1:1:2547:G:H1'     | 2.20                     | 0.40              |
| 1:1:2646:A:C2      | 13:s:124:GLY:HA3   | 2.57                     | 0.40              |
| 1:1:2771:A:H5''    | 1:1:2772:G:O5'     | 2.21                     | 0.40              |
| 1:1:3109:C:H5''    | 5:k:276:THR:HB     | 2.02                     | 0.40              |
| 2:3:82:G:C6        | 2:3:99:G:C6        | 3.09                     | 0.40              |
| 14:t:134:GLU:O     | 14:t:138:PHE:CD2   | 2.74                     | 0.40              |
| 15:u:116:LEU:HD13  | 17:w:194:LYS:HB2   | 2.03                     | 0.40              |
| 19:y:147:ARG:HB3   | 19:y:150:VAL:HG23  | 2.02                     | 0.40              |
| 34:AG:7:LEU:HD23   | 34:AG:7:LEU:HA     | 1.94                     | 0.40              |
| 45:i:65:LYS:HE3    | 65:U:120:ARG:HH11  | 1.86                     | 0.40              |
| 46:B:94:U:O2'      | 51:G:7:LYS:HB2     | 2.21                     | 0.40              |
| 46:B:326:A:H2'     | 46:B:327:G:O4'     | 2.22                     | 0.40              |
| 46:B:327:G:H2'     | 46:B:328:G:C8      | 2.56                     | 0.40              |
| 46:B:364:A:C2      | 46:B:374:C:C2      | 3.09                     | 0.40              |
| 46:B:443:A:C2      | 46:B:444:A:C8      | 3.09                     | 0.40              |
| 46:B:461:U:H2'     | 46:B:462:A:C8      | 2.56                     | 0.40              |
| 46:B:1157:G:H2'    | 46:B:1158:C:O4'    | 2.22                     | 0.40              |
| 46:B:1378:U:H2'    | 46:B:1379:C:H6     | 1.86                     | 0.40              |
| 50:F:8:LYS:HD3     | 50:F:8:LYS:HA      | 1.83                     | 0.40              |
| 50:F:21:GLU:HG3    | 57:M:61:TRP:CG     | 2.56                     | 0.40              |
| 60:P:25:TRP:CE3    | 74:d:82:LYS:HE3    | 2.56                     | 0.40              |
| 62:R:14:GLN:OE1    | 62:R:21:ASP:HB2    | 2.21                     | 0.40              |
| 1:AS:206:U:H2'     | 1:AS:207:C:C6      | 2.57                     | 0.40              |
| 1:AS:438:A:C8      | 33:BZ:3:THR:HG23   | 2.57                     | 0.40              |
| 1:AS:756:G:H1'     | 1:AS:767:A:N6      | 2.37                     | 0.40              |
| 1:AS:803:A:C2      | 1:AS:804:A:C8      | 3.10                     | 0.40              |
| 1:AS:1034:U:H2'    | 1:AS:1035:U:C6     | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AS:1075:A:C2     | 7:AZ:113:LEU:HD22  | 2.56                     | 0.40              |
| 1:AS:1165:A:H5'    | 9:BB:212:PHE:HD2   | 1.86                     | 0.40              |
| 1:AS:1203:G:H4'    | 41:CH:41:HIS:O     | 2.22                     | 0.40              |
| 11:BD:180:TYR:CD1  | 41:CH:13:TYR:HD2   | 2.38                     | 0.40              |
| 19:BL:175:ALA:HB3  | 29:BV:53:PHE:O     | 2.21                     | 0.40              |
| 25:BR:50:SER:HA    | 25:BR:55:TYR:CD2   | 2.55                     | 0.40              |
| 32:BY:82:GLU:O     | 32:BY:83:ASP:HB3   | 2.22                     | 0.40              |
| 45:CL:66:ASN:O     | 45:CL:67:LYS:HD3   | 2.21                     | 0.40              |
| 46:CM:181:U:H2'    | 46:CM:182:C:C6     | 2.57                     | 0.40              |
| 46:CM:857:G:H22    | 46:CM:1032:G:H4'   | 1.85                     | 0.40              |
| 46:CM:917:U:OP2    | 48:CO:117:TRP:N    | 2.53                     | 0.40              |
| 46:CM:985:C:H6     | 46:CM:988:A:C8     | 2.40                     | 0.40              |
| 46:CM:1215:A:H2    | 46:CM:1243:U:C2    | 2.39                     | 0.40              |
| 46:CM:1579:A:O2'   | 46:CM:1580:A:OP1   | 2.35                     | 0.40              |
| 47:CN:117:GLU:O    | 49:CP:35:LYS:HE2   | 2.21                     | 0.40              |
| 51:CR:247:LEU:HB3  | 51:CR:251:GLU:HB2  | 2.03                     | 0.40              |
| 58:CY:28:ASN:O     | 58:CY:30:LYS:N     | 2.45                     | 0.40              |
| 61:DB:105:LEU:HD23 | 61:DB:105:LEU:HA   | 1.93                     | 0.40              |
| 62:DC:68:GLU:HB2   | 62:DC:69:PRO:HD3   | 2.02                     | 0.40              |
| 62:DC:85:VAL:HB    | 62:DC:112:VAL:HA   | 2.03                     | 0.40              |
| 70:DK:109:ARG:HD3  | 70:DK:113:ALA:O    | 2.21                     | 0.40              |
| 73:DN:12:LYS:HA    | 73:DN:15:ARG:NH1   | 2.36                     | 0.40              |
| 79:DT:21:THR:OG1   | 79:DT:22:SER:N     | 2.54                     | 0.40              |
| 79:DT:237:VAL:HA   | 79:DT:253:THR:HG22 | 2.02                     | 0.40              |
| 81:P0:16:ARG:HD2   | 81:P0:66:PHE:CE2   | 2.56                     | 0.40              |
| 82:12:121:PHE:O    | 82:12:122:GLY:C    | 2.65                     | 0.40              |
| 1:1:88:G:H21       | 1:1:281:G:H4'      | 1.86                     | 0.40              |
| 1:1:99:A:H3'       | 1:1:100:G:H21      | 1.87                     | 0.40              |
| 1:1:675:A:H4'      | 1:1:676:G:O5'      | 2.21                     | 0.40              |
| 1:1:1241:A:H3'     | 1:1:1242:G:C5'     | 2.49                     | 0.40              |
| 1:1:1358:C:H2'     | 1:1:1359:A:H8      | 1.86                     | 0.40              |
| 1:1:1485:A:OP1     | 35:AH:10:ARG:HD2   | 2.21                     | 0.40              |
| 1:1:1591:U:C2      | 1:1:1592:C:C5      | 3.09                     | 0.40              |
| 1:1:1644:A:H2'     | 1:1:1645:U:O4'     | 2.22                     | 0.40              |
| 1:1:2680:C:H2'     | 1:1:2681:C:H6      | 1.86                     | 0.40              |
| 1:1:2984:A:N1      | 1:1:3015:C:C2      | 2.90                     | 0.40              |
| 1:1:3061:C:H2'     | 1:1:3062:U:O4'     | 2.21                     | 0.40              |
| 4:j:245:LEU:HD12   | 4:j:245:LEU:HA     | 1.96                     | 0.40              |
| 24:6:36:VAL:HG22   | 24:6:58:VAL:HG11   | 2.04                     | 0.40              |
| 24:6:38:ALA:O      | 24:6:58:VAL:HG13   | 2.21                     | 0.40              |
| 28:AA:14:VAL:HG22  | 28:AA:79:HIS:O     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:AE:18:ARG:HD3  | 32:AE:34:GLU:HB3  | 2.02                     | 0.40              |
| 46:B:591:A:OP1    | 56:L:40:ARG:HB2   | 2.22                     | 0.40              |
| 46:B:598:U:P      | 70:Z:108:GLY:HA2  | 2.61                     | 0.40              |
| 46:B:736:G:H2'    | 46:B:737:A:H8     | 1.86                     | 0.40              |
| 46:B:1003:U:OP1   | 60:P:107:LYS:NZ   | 2.53                     | 0.40              |
| 46:B:1070:G:H2'   | 46:B:1072:A:OP2   | 2.21                     | 0.40              |
| 46:B:1118:A:H2'   | 46:B:1119:C:O4'   | 2.21                     | 0.40              |
| 46:B:1460:G:C2    | 46:B:1461:A:C5    | 3.09                     | 0.40              |
| 46:B:1589:C:H2'   | 46:B:1590:U:H6    | 1.86                     | 0.40              |
| 46:B:1725:U:H2'   | 46:B:1726:C:C6    | 2.56                     | 0.40              |
| 49:E:97:VAL:HG11  | 49:E:124:ILE:CG1  | 2.51                     | 0.40              |
| 50:F:69:GLU:HA    | 57:M:90:THR:HB    | 2.04                     | 0.40              |
| 52:H:148:ARG:HB3  | 52:H:157:ARG:NH1  | 2.37                     | 0.40              |
| 52:H:213:LYS:HD3  | 52:H:213:LYS:HA   | 1.71                     | 0.40              |
| 55:K:141:ARG:HB2  | 55:K:146:GLU:HG3  | 2.02                     | 0.40              |
| 58:N:44:THR:HG23  | 58:N:60:PHE:CD1   | 2.56                     | 0.40              |
| 59:O:76:GLU:OE2   | 59:O:90:LYS:HE2   | 2.22                     | 0.40              |
| 61:Q:12:ALA:HB3   | 61:Q:76:ILE:HD13  | 2.03                     | 0.40              |
| 63:S:98:GLU:HB2   | 79:AR:60:LYS:HA   | 2.03                     | 0.40              |
| 69:Y:55:ASP:OD1   | 69:Y:55:ASP:N     | 2.54                     | 0.40              |
| 69:Y:77:PRO:HD3   | 70:Z:7:ARG:O      | 2.21                     | 0.40              |
| 75:e:60:GLU:H     | 75:e:60:GLU:CD    | 2.28                     | 0.40              |
| 1:AS:74:G:H5'     | 14:BG:58:VAL:HB   | 2.03                     | 0.40              |
| 1:AS:78:U:C2      | 1:AS:79:G:C8      | 3.10                     | 0.40              |
| 1:AS:844:A:C6     | 1:AS:845:C:H1'    | 2.56                     | 0.40              |
| 1:AS:1011:C:H42   | 1:AS:1031:A:N6    | 2.19                     | 0.40              |
| 1:AS:1210:U:H2'   | 1:AS:1211:U:C6    | 2.56                     | 0.40              |
| 1:AS:1329:C:O2'   | 9:BB:205:LEU:O    | 2.38                     | 0.40              |
| 1:AS:1521:G:N3    | 1:AS:1521:G:H2'   | 2.35                     | 0.40              |
| 1:AS:1645:U:H3    | 1:AS:1802:A:H61   | 1.70                     | 0.40              |
| 1:AS:1921:U:C1'   | 44:CK:20:SER:HB3  | 2.51                     | 0.40              |
| 1:AS:2779:U:O3'   | 1:AS:2780:A:H3'   | 2.20                     | 0.40              |
| 2:AT:1:G:C4       | 7:AZ:266:LYS:HA   | 2.55                     | 0.40              |
| 10:BC:94:LEU:HD12 | 10:BC:94:LEU:HA   | 1.70                     | 0.40              |
| 10:BC:173:LYS:HE2 | 10:BC:173:LYS:HB2 | 1.87                     | 0.40              |
| 11:BD:2:LYS:HA    | 11:BD:2:LYS:HD2   | 1.94                     | 0.40              |
| 11:BD:94:TYR:HA   | 11:BD:177:ASP:OD1 | 2.21                     | 0.40              |
| 16:BI:56:LYS:HE3  | 16:BI:56:LYS:HB3  | 1.81                     | 0.40              |
| 21:BN:27:MET:HB3  | 21:BN:27:MET:HE2  | 1.80                     | 0.40              |
| 27:BT:112:ASP:OD1 | 27:BT:115:ARG:HG2 | 2.21                     | 0.40              |
| 34:CA:52:VAL:HG22 | 34:CA:66:VAL:HG12 | 2.02                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:CB:58:ARG:CD    | 35:CB:59:PRO:HD2   | 2.35                     | 0.40              |
| 46:CM:66:U:O2      | 53:CT:160:ARG:NE   | 2.47                     | 0.40              |
| 46:CM:520:U:H5''   | 71:DL:37:LYS:HG3   | 2.04                     | 0.40              |
| 46:CM:1019:C:OP1   | 60:DA:9:LYS:NZ     | 2.31                     | 0.40              |
| 46:CM:1071:A:H2'   | 46:CM:1072:A:C8    | 2.56                     | 0.40              |
| 46:CM:1219:A:H5'   | 46:CM:1220:C:OP1   | 2.21                     | 0.40              |
| 46:CM:1469:A:H4'   | 63:DD:70:GLY:HA2   | 2.04                     | 0.40              |
| 52:CS:83:ARG:HA    | 52:CS:86:GLN:HG3   | 2.03                     | 0.40              |
| 54:CU:47:VAL:HG21  | 54:CU:167:GLN:CG   | 2.51                     | 0.40              |
| 59:CZ:54:LYS:C     | 59:CZ:56:GLU:H     | 2.29                     | 0.40              |
| 59:CZ:108:ARG:O    | 59:CZ:108:ARG:HG3  | 2.22                     | 0.40              |
| 61:DB:117:PRO:CB   | 61:DB:120:SER:HB3  | 2.51                     | 0.40              |
| 65:DF:101:LEU:HD23 | 65:DF:101:LEU:HA   | 1.87                     | 0.40              |
| 67:DH:101:ARG:O    | 67:DH:105:ILE:HG12 | 2.20                     | 0.40              |
| 79:DT:194:GLY:N    | 79:DT:214:ASP:HB3  | 2.25                     | 0.40              |
| 1:1:48:A:N7        | 16:v:187:ARG:HD2   | 2.37                     | 0.40              |
| 1:1:224:C:H5'      | 27:9:34:PRO:HD3    | 2.03                     | 0.40              |
| 1:1:530:U:O2       | 21:0:146:LYS:HA    | 2.22                     | 0.40              |
| 1:1:640:U:H2'      | 1:1:642:G:OP2      | 2.22                     | 0.40              |
| 1:1:744:U:H2'      | 1:1:745:C:C6       | 2.56                     | 0.40              |
| 1:1:823:A:H2'      | 1:1:824:A:H8       | 1.85                     | 0.40              |
| 1:1:903:G:C5       | 1:1:922:A:C8       | 3.10                     | 0.40              |
| 1:1:1034:U:O3'     | 7:m:5:LYS:HA       | 2.20                     | 0.40              |
| 1:1:1676:G:H2'     | 1:1:1677:U:H6      | 1.86                     | 0.40              |
| 1:1:2325:U:H2'     | 1:1:2326:A:O4'     | 2.22                     | 0.40              |
| 1:1:2913:A:O5'     | 1:1:2915:G:H4'     | 2.22                     | 0.40              |
| 1:1:3172:U:O4      | 21:0:159:SER:HB3   | 2.21                     | 0.40              |
| 2:3:90:A:H2'       | 2:3:91:G:O4'       | 2.22                     | 0.40              |
| 5:k:112:GLU:O      | 5:k:116:ARG:HG3    | 2.21                     | 0.40              |
| 11:q:150:SER:OG    | 11:q:153:ALA:HB3   | 2.21                     | 0.40              |
| 14:t:42:LYS:HE3    | 14:t:51:ILE:HB     | 2.04                     | 0.40              |
| 30:AC:21:ILE:O     | 30:AC:21:ILE:HG22  | 2.22                     | 0.40              |
| 35:AH:20:ILE:HG22  | 35:AH:34:HIS:CD2   | 2.56                     | 0.40              |
| 38:AK:44:MET:HE3   | 38:AK:44:MET:HB3   | 1.84                     | 0.40              |
| 46:B:160:A:C6      | 46:B:161:G:C6      | 3.09                     | 0.40              |
| 46:B:512:G:N3      | 46:B:513:A:C8      | 2.90                     | 0.40              |
| 46:B:558:U:H2'     | 46:B:559:G:C8      | 2.52                     | 0.40              |
| 46:B:740:A:HO2'    | 46:B:741:A:P       | 2.43                     | 0.40              |
| 46:B:783:A:H4'     | 51:G:201:HIS:CE1   | 2.56                     | 0.40              |
| 46:B:814:A:H2      | 46:B:815:U:N3      | 2.19                     | 0.40              |
| 46:B:1436:U:H2'    | 46:B:1437:C:C6     | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:B:1494:G:H2'   | 46:B:1495:U:C6     | 2.56                     | 0.40              |
| 46:B:1744:G:O6    | 86:B:1851:GET:H621 | 2.21                     | 0.40              |
| 47:C:88:LYS:NZ    | 64:T:82:ASP:O      | 2.42                     | 0.40              |
| 47:C:90:ALA:HB2   | 47:C:97:ALA:HB2    | 2.02                     | 0.40              |
| 48:D:180:THR:HG22 | 48:D:183:GLN:OE1   | 2.22                     | 0.40              |
| 51:G:12:LEU:HD23  | 51:G:12:LEU:HA     | 1.89                     | 0.40              |
| 53:I:136:LYS:O    | 53:I:175:ILE:HA    | 2.21                     | 0.40              |
| 56:L:100:LYS:HB3  | 56:L:102:GLU:OE1   | 2.22                     | 0.40              |
| 59:O:53:SER:HA    | 78:h:158:ARG:HH21  | 1.87                     | 0.40              |
| 1:AS:173:C:H2'    | 1:AS:174:C:C6      | 2.55                     | 0.40              |
| 1:AS:976:A:H3'    | 1:AS:976:A:C8      | 2.57                     | 0.40              |
| 1:AS:1560:U:H2'   | 1:AS:1561:U:C6     | 2.56                     | 0.40              |
| 1:AS:2236:U:H2'   | 1:AS:2237:A:H8     | 1.86                     | 0.40              |
| 1:AS:2257:A:C8    | 1:AS:2266:G:C8     | 3.09                     | 0.40              |
| 1:AS:2497:A:H2'   | 1:AS:2498:A:C8     | 2.56                     | 0.40              |
| 1:AS:2650:A:P     | 45:CL:57:PRO:HD2   | 2.61                     | 0.40              |
| 1:AS:2681:C:H2'   | 1:AS:2682:C:C6     | 2.56                     | 0.40              |
| 1:AS:2814:U:N3    | 1:AS:2815:U:C5     | 2.90                     | 0.40              |
| 3:AU:4:C:H5'      | 18:BK:61:ARG:HB3   | 2.04                     | 0.40              |
| 3:AU:38:U:O2      | 36:CC:83:LYS:HB2   | 2.21                     | 0.40              |
| 4:AW:107:CYS:O    | 4:AW:139:HIS:NE2   | 2.45                     | 0.40              |
| 5:AX:47:LEU:HD23  | 5:AX:47:LEU:HA     | 1.94                     | 0.40              |
| 5:AX:58:ARG:CD    | 5:AX:354:VAL:HG13  | 2.49                     | 0.40              |
| 5:AX:140:ASP:OD1  | 5:AX:140:ASP:N     | 2.52                     | 0.40              |
| 6:AY:301:ARG:HG2  | 19:BL:39:ARG:O     | 2.22                     | 0.40              |
| 7:AZ:182:GLY:CA   | 7:AZ:194:LEU:HD22  | 2.52                     | 0.40              |
| 80:BE:50:ILE:HG21 | 80:BE:149:ILE:HD13 | 2.04                     | 0.40              |
| 80:BE:86:HIS:HB3  | 80:BE:139:ARG:CG   | 2.52                     | 0.40              |
| 13:BF:87:LYS:HB2  | 13:BF:87:LYS:HE2   | 1.81                     | 0.40              |
| 14:BG:75:PHE:HA   | 14:BG:101:ARG:HH21 | 1.87                     | 0.40              |
| 15:BH:19:VAL:HG12 | 15:BH:57:LEU:HA    | 2.03                     | 0.40              |
| 17:BJ:9:VAL:HG12  | 17:BJ:118:ARG:HG3  | 2.03                     | 0.40              |
| 19:BL:69:ARG:HG3  | 19:BL:69:ARG:HH11  | 1.86                     | 0.40              |
| 25:BR:102:LYS:CD  | 25:BR:105:ARG:HH22 | 2.35                     | 0.40              |
| 42:CI:2:ARG:HB3   | 42:CI:5:TRP:CD1    | 2.57                     | 0.40              |
| 46:CM:115:G:H5'   | 58:CY:129:ARG:HD3  | 2.03                     | 0.40              |
| 46:CM:126:A:OP1   | 53:CT:201:GLN:HG3  | 2.21                     | 0.40              |
| 46:CM:184:C:P     | 55:CV:152:ARG:HH22 | 2.42                     | 0.40              |
| 46:CM:217:A:P     | 46:CM:816:U:H1'    | 2.62                     | 0.40              |
| 46:CM:404:U:H2'   | 46:CM:405:A:H8     | 1.86                     | 0.40              |
| 46:CM:433:C:OP2   | 70:DK:77:ILE:HD11  | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:CM:501:G:P     | 46:CM:501:G:H8    | 2.45                     | 0.40              |
| 46:CM:617:A:H5'   | 46:CM:618:A:OP2   | 2.22                     | 0.40              |
| 46:CM:654:G:H5''  | 46:CM:655:U:OP2   | 2.22                     | 0.40              |
| 46:CM:740:A:O2'   | 46:CM:741:A:OP1   | 2.32                     | 0.40              |
| 46:CM:885:A:H2'   | 46:CM:886:G:C8    | 2.55                     | 0.40              |
| 47:CN:55:GLU:HB3  | 68:DI:79:LEU:HD22 | 2.02                     | 0.40              |
| 53:CT:141:ILE:O   | 53:CT:145:PHE:HD2 | 2.03                     | 0.40              |
| 54:CU:107:LYS:HE3 | 54:CU:107:LYS:HB3 | 1.86                     | 0.40              |
| 59:CZ:85:LYS:O    | 59:CZ:86:ILE:C    | 2.64                     | 0.40              |
| 62:DC:27:GLU:O    | 62:DC:28:MET:C    | 2.65                     | 0.40              |
| 79:DT:118:LYS:HA  | 79:DT:118:LYS:CE  | 2.45                     | 0.40              |
| 79:DT:270:GLU:C   | 79:DT:272:LYS:N   | 2.78                     | 0.40              |
| 81:P0:97:ARG:HA   | 81:P0:100:VAL:CG2 | 2.51                     | 0.40              |
| 1:1:1153:G:O2'    | 1:1:1165:A:N3     | 2.44                     | 0.40              |
| 1:1:1231:U:H1'    | 1:1:1233:G:OP2    | 2.21                     | 0.40              |
| 1:1:1496:G:H2'    | 1:1:1497:U:O4'    | 2.21                     | 0.40              |
| 1:1:1654:G:C5     | 1:1:1792:G:C6     | 3.09                     | 0.40              |
| 1:1:1756:A:C6     | 1:1:1762:G:C5     | 3.10                     | 0.40              |
| 1:1:1866:C:H5''   | 1:1:3048:C:O2'    | 2.22                     | 0.40              |
| 1:1:1937:C:H2'    | 1:1:1938:U:C6     | 2.57                     | 0.40              |
| 1:1:2640:U:H5''   | 45:i:50:LYS:NZ    | 2.37                     | 0.40              |
| 1:1:3035:C:H2'    | 1:1:3036:U:C6     | 2.57                     | 0.40              |
| 1:1:3153:A:H2'    | 1:1:3154:A:H8     | 1.85                     | 0.40              |
| 4:j:112:ILE:HG13  | 44:AQ:79:VAL:HG22 | 2.03                     | 0.40              |
| 5:k:99:LEU:HD23   | 5:k:99:LEU:HA     | 1.92                     | 0.40              |
| 7:m:7:PHE:C       | 7:m:7:PHE:CD1     | 2.99                     | 0.40              |
| 7:m:178:ASN:HA    | 7:m:183:TRP:CG    | 2.56                     | 0.40              |
| 9:o:186:ILE:HD11  | 9:o:196:VAL:HG12  | 2.03                     | 0.40              |
| 16:v:46:ASP:OD2   | 16:v:50:ARG:NH2   | 2.48                     | 0.40              |
| 21:0:119:ARG:H    | 21:0:119:ARG:HG3  | 1.59                     | 0.40              |
| 24:6:80:ARG:HG2   | 24:6:99:ALA:HB3   | 2.04                     | 0.40              |
| 25:7:124:LYS:HD2  | 25:7:124:LYS:C    | 2.46                     | 0.40              |
| 29:AB:126:LYS:HA  | 29:AB:146:GLU:O   | 2.22                     | 0.40              |
| 33:AF:35:LYS:HE3  | 33:AF:53:GLN:OE1  | 2.21                     | 0.40              |
| 37:AJ:57:ILE:HG23 | 37:AJ:93:ILE:HD11 | 2.04                     | 0.40              |
| 42:AO:7:LYS:HD3   | 42:AO:11:ARG:NH2  | 2.36                     | 0.40              |
| 45:i:103:LEU:HD22 | 50:F:149:LYS:NZ   | 2.37                     | 0.40              |
| 46:B:57:G:OP2     | 71:a:116:LYS:HD3  | 2.21                     | 0.40              |
| 46:B:214:U:H2'    | 46:B:214:U:OP2    | 2.21                     | 0.40              |
| 46:B:585:C:C4     | 46:B:586:U:C4     | 3.10                     | 0.40              |
| 46:B:1146:C:H2'   | 46:B:1147:C:H6    | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:B:1533:G:P      | 65:U:123:ARG:HH11  | 2.44                     | 0.40              |
| 51:G:94:ALA:HB3    | 71:a:17:LEU:HD23   | 2.03                     | 0.40              |
| 57:M:5:LYS:HZ2     | 59:O:38:HIS:CE1    | 2.39                     | 0.40              |
| 57:M:26:ASP:CG     | 57:M:29:GLN:HB2    | 2.47                     | 0.40              |
| 62:R:90:ILE:HD11   | 62:R:112:VAL:HG21  | 2.03                     | 0.40              |
| 64:T:7:LYS:O       | 64:T:11:ARG:HG2    | 2.21                     | 0.40              |
| 64:T:11:ARG:O      | 64:T:15:VAL:HG23   | 2.20                     | 0.40              |
| 67:W:24:THR:HB     | 67:W:114:GLU:HG3   | 2.04                     | 0.40              |
| 79:AR:47:LEU:HD12  | 79:AR:55:TYR:CD1   | 2.56                     | 0.40              |
| 79:AR:64:GLY:O     | 79:AR:91:ARG:NH1   | 2.55                     | 0.40              |
| 1:AS:426:G:H2'     | 1:AS:427:C:H6      | 1.86                     | 0.40              |
| 1:AS:533:G:H2'     | 1:AS:534:G:O4'     | 2.21                     | 0.40              |
| 1:AS:538:G:O2'     | 1:AS:539:G:OP1     | 2.38                     | 0.40              |
| 1:AS:741:C:H2'     | 1:AS:742:C:H6      | 1.85                     | 0.40              |
| 1:AS:1009:G:H21    | 7:AZ:3:MET:CE      | 2.34                     | 0.40              |
| 1:AS:1217:A:H4'    | 1:AS:1218:G:OP2    | 2.21                     | 0.40              |
| 1:AS:1295:U:H2'    | 1:AS:1296:G:O4'    | 2.22                     | 0.40              |
| 1:AS:1537:G:H1'    | 1:AS:1553:A:C4     | 2.57                     | 0.40              |
| 1:AS:1684:U:O4     | 23:BP:77:LYS:HE2   | 2.21                     | 0.40              |
| 1:AS:1705:C:C2     | 1:AS:1706:C:C5     | 3.09                     | 0.40              |
| 1:AS:2185:A:C6     | 46:CM:898:G:C2     | 3.09                     | 0.40              |
| 1:AS:2276:U:O2'    | 1:AS:2277:A:H5'    | 2.21                     | 0.40              |
| 1:AS:2407:G:H2'    | 1:AS:2408:A:C8     | 2.57                     | 0.40              |
| 1:AS:2413:G:N7     | 1:AS:2565:A:H2'    | 2.36                     | 0.40              |
| 1:AS:2603:U:H4'    | 1:AS:2669:A:C2     | 2.57                     | 0.40              |
| 1:AS:2646:A:H5''   | 13:BF:105:GLY:HA3  | 2.03                     | 0.40              |
| 1:AS:3212:G:H2'    | 1:AS:3213:C:C6     | 2.56                     | 0.40              |
| 2:AT:45:A:H2'      | 2:AT:46:A:H8       | 1.86                     | 0.40              |
| 4:AW:30:ARG:HG2    | 4:AW:74:GLU:HG3    | 2.04                     | 0.40              |
| 4:AW:101:ILE:CG1   | 4:AW:165:VAL:HG22  | 2.51                     | 0.40              |
| 6:AY:356:GLN:HE22  | 22:BO:147:ILE:HG12 | 1.86                     | 0.40              |
| 10:BC:162:GLU:HA   | 10:BC:165:VAL:HG12 | 2.02                     | 0.40              |
| 14:BG:37:GLN:HA    | 14:BG:40:LEU:HD12  | 2.02                     | 0.40              |
| 16:BI:68:ARG:HG2   | 16:BI:128:LYS:HG3  | 2.04                     | 0.40              |
| 20:BM:10:LEU:HD23  | 20:BM:10:LEU:HA    | 1.81                     | 0.40              |
| 22:BO:124:GLU:HG3  | 22:BO:125:THR:N    | 2.36                     | 0.40              |
| 23:BP:18:ASP:O     | 23:BP:108:LEU:HD12 | 2.22                     | 0.40              |
| 28:BU:84:ARG:NH1   | 28:BU:85:TYR:CZ    | 2.90                     | 0.40              |
| 31:BX:11:ASN:HB3   | 31:BX:12:ILE:HD12  | 2.04                     | 0.40              |
| 31:BX:29:TYR:OH    | 31:BX:57:GLU:OE2   | 2.36                     | 0.40              |
| 36:CC:118:ILE:HG22 | 36:CC:119:LYS:N    | 2.37                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:CD:52:TYR:O    | 37:CD:56:LEU:HD12  | 2.22                     | 0.40              |
| 46:CM:509:A:H5'   | 56:CW:173:LYS:HB2  | 2.03                     | 0.40              |
| 46:CM:695:C:H42   | 54:CU:103:ARG:NH2  | 2.19                     | 0.40              |
| 46:CM:800:G:C2    | 46:CM:801:A:C8     | 3.09                     | 0.40              |
| 46:CM:935:C:H2'   | 46:CM:936:A:C8     | 2.57                     | 0.40              |
| 48:CO:111:ARG:HB3 | 73:DN:68:TYR:HB2   | 2.03                     | 0.40              |
| 51:CR:152:PRO:HD2 | 53:CT:211:LEU:CD2  | 2.52                     | 0.40              |
| 51:CR:176:ASP:HB3 | 51:CR:179:ARG:NH1  | 2.36                     | 0.40              |
| 52:CS:84:LYS:HE3  | 52:CS:84:LYS:HB3   | 1.78                     | 0.40              |
| 56:CW:68:LYS:HE2  | 56:CW:68:LYS:HB3   | 1.92                     | 0.40              |
| 57:CX:7:ASP:O     | 57:CX:11:ILE:HG13  | 2.22                     | 0.40              |
| 62:DC:33:PHE:CZ   | 62:DC:112:VAL:HG22 | 2.56                     | 0.40              |
| 67:DH:43:ASN:HD21 | 67:DH:105:ILE:CG2  | 2.33                     | 0.40              |
| 79:DT:59:LYS:HA   | 79:DT:59:LYS:HD3   | 1.94                     | 0.40              |
| 81:P0:71:PRO:O    | 81:P0:72:GLU:C     | 2.64                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | AW    | 247/254 (97%) | 240 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 4   | j     | 247/254 (97%) | 239 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 5   | AX    | 384/389 (99%) | 372 (97%) | 12 (3%) | 0        | 100         | 100 |
| 5   | k     | 384/389 (99%) | 374 (97%) | 9 (2%)  | 1 (0%)   | 36          | 67  |
| 6   | AY    | 357/363 (98%) | 349 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 6   | l     | 357/363 (98%) | 346 (97%) | 10 (3%) | 1 (0%)   | 36          | 67  |
| 7   | AZ    | 290/298 (97%) | 280 (97%) | 10 (3%) | 0        | 100         | 100 |
| 7   | m     | 292/298 (98%) | 281 (96%) | 11 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8   | BA    | 149/176 (85%) | 147 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 8   | n     | 153/176 (87%) | 150 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 9   | BB    | 224/241 (93%) | 218 (97%) | 5 (2%)   | 1 (0%)   | 30          | 62  |
| 9   | o     | 227/241 (94%) | 220 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 10  | BC    | 231/262 (88%) | 210 (91%) | 16 (7%)  | 5 (2%)   | 5           | 30  |
| 10  | p     | 234/262 (89%) | 225 (96%) | 8 (3%)   | 1 (0%)   | 30          | 62  |
| 11  | BD    | 188/191 (98%) | 182 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 11  | q     | 188/191 (98%) | 182 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 12  | r     | 203/219 (93%) | 201 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 13  | BF    | 169/174 (97%) | 162 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 13  | s     | 169/174 (97%) | 161 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 14  | BG    | 198/202 (98%) | 179 (90%) | 12 (6%)  | 7 (4%)   | 3           | 23  |
| 14  | t     | 198/202 (98%) | 196 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 15  | BH    | 128/131 (98%) | 124 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 15  | u     | 126/131 (96%) | 123 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 16  | BI    | 201/204 (98%) | 198 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 16  | v     | 201/204 (98%) | 196 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 17  | BJ    | 197/200 (98%) | 195 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 17  | w     | 197/200 (98%) | 195 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 18  | BK    | 170/185 (92%) | 166 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 18  | x     | 165/185 (89%) | 160 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 19  | BL    | 183/186 (98%) | 179 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 19  | y     | 183/186 (98%) | 179 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 20  | BM    | 177/190 (93%) | 174 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 20  | z     | 177/190 (93%) | 172 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 21  | 0     | 168/172 (98%) | 166 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 21  | BN    | 168/172 (98%) | 166 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 22  | 2     | 157/160 (98%) | 153 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 22  | BO    | 157/160 (98%) | 153 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 23  | 5     | 98/124 (79%)  | 90 (92%)  | 6 (6%)   | 2 (2%)   | 6           | 32  |
| 23  | BP    | 97/124 (78%)  | 75 (77%)  | 16 (16%) | 6 (6%)   | 1           | 12  |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 24  | 6     | 129/137 (94%) | 126 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 24  | BQ    | 129/137 (94%) | 126 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 25  | 7     | 114/155 (74%) | 89 (78%)   | 25 (22%) | 0        | 100         | 100 |
| 25  | BR    | 105/155 (68%) | 90 (86%)   | 14 (13%) | 1 (1%)   | 12          | 44  |
| 26  | 8     | 118/142 (83%) | 117 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 26  | BS    | 117/142 (82%) | 111 (95%)  | 5 (4%)   | 1 (1%)   | 14          | 47  |
| 27  | 9     | 124/127 (98%) | 120 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 27  | BT    | 124/127 (98%) | 123 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 28  | AA    | 133/136 (98%) | 132 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 28  | BU    | 133/136 (98%) | 116 (87%)  | 15 (11%) | 2 (2%)   | 8           | 37  |
| 29  | AB    | 146/149 (98%) | 138 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 29  | BV    | 146/149 (98%) | 139 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 30  | AC    | 56/63 (89%)   | 52 (93%)   | 1 (2%)   | 3 (5%)   | 1           | 14  |
| 30  | BW    | 58/63 (92%)   | 57 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 31  | AD    | 96/106 (91%)  | 92 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 31  | BX    | 92/106 (87%)  | 90 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 32  | AE    | 106/112 (95%) | 104 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 32  | BY    | 106/112 (95%) | 103 (97%)  | 2 (2%)   | 1 (1%)   | 14          | 47  |
| 33  | AF    | 122/131 (93%) | 121 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 33  | BZ    | 120/131 (92%) | 120 (100%) | 0        | 0        | 100         | 100 |
| 34  | AG    | 104/107 (97%) | 101 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 34  | CA    | 104/107 (97%) | 101 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 35  | AH    | 110/122 (90%) | 108 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 35  | CB    | 108/122 (88%) | 105 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 36  | AI    | 113/120 (94%) | 112 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 36  | CC    | 115/120 (96%) | 111 (96%)  | 3 (3%)   | 1 (1%)   | 14          | 47  |
| 37  | AJ    | 95/99 (96%)   | 94 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 37  | CD    | 93/99 (94%)   | 85 (91%)   | 8 (9%)   | 0        | 100         | 100 |
| 38  | AK    | 84/90 (93%)   | 80 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 38  | CE    | 84/90 (93%)   | 81 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 39  | AL    | 75/78 (96%)   | 70 (93%)   | 5 (7%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 39  | CF    | 75/78 (96%)   | 65 (87%)   | 7 (9%)   | 3 (4%)   | 2           | 19  |
| 40  | AM    | 48/51 (94%)   | 48 (100%)  | 0        | 0        | 100         | 100 |
| 40  | CG    | 48/51 (94%)   | 47 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 41  | AN    | 48/52 (92%)   | 48 (100%)  | 0        | 0        | 100         | 100 |
| 41  | CH    | 48/52 (92%)   | 46 (96%)   | 1 (2%)   | 1 (2%)   | 5           | 31  |
| 42  | AO    | 23/25 (92%)   | 22 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 42  | CI    | 22/25 (88%)   | 22 (100%)  | 0        | 0        | 100         | 100 |
| 43  | AP    | 101/106 (95%) | 99 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 43  | CJ    | 101/106 (95%) | 99 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 44  | AQ    | 89/92 (97%)   | 85 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 44  | CK    | 89/92 (97%)   | 85 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 45  | CL    | 116/267 (43%) | 72 (62%)   | 34 (29%) | 10 (9%)  | 0           | 7   |
| 45  | i     | 104/267 (39%) | 51 (49%)   | 35 (34%) | 18 (17%) | 0           | 2   |
| 47  | C     | 206/261 (79%) | 200 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 47  | CN    | 206/261 (79%) | 199 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 48  | CO    | 211/256 (82%) | 191 (90%)  | 14 (7%)  | 6 (3%)   | 4           | 26  |
| 48  | D     | 212/256 (83%) | 207 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 49  | CP    | 215/249 (86%) | 209 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 49  | E     | 215/249 (86%) | 208 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 50  | CQ    | 221/251 (88%) | 211 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 50  | F     | 221/251 (88%) | 214 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 51  | CR    | 258/262 (98%) | 255 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 51  | G     | 256/262 (98%) | 252 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 52  | CS    | 203/225 (90%) | 180 (89%)  | 20 (10%) | 3 (2%)   | 8           | 37  |
| 52  | H     | 204/225 (91%) | 193 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 53  | CT    | 234/236 (99%) | 228 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 53  | I     | 221/236 (94%) | 217 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 54  | CU    | 177/186 (95%) | 150 (85%)  | 21 (12%) | 6 (3%)   | 3           | 23  |
| 54  | J     | 180/186 (97%) | 171 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 55  | CV    | 201/206 (98%) | 199 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 55  | K     | 201/206 (98%) | 200 (100%) | 1 (0%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 56  | CW    | 176/189 (93%) | 174 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 56  | L     | 176/189 (93%) | 175 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 57  | CX    | 92/118 (78%)  | 86 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 57  | M     | 96/118 (81%)  | 82 (85%)   | 12 (12%) | 2 (2%)   | 5           | 31  |
| 58  | CY    | 139/155 (90%) | 133 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 58  | N     | 142/155 (92%) | 136 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 59  | CZ    | 117/143 (82%) | 75 (64%)   | 36 (31%) | 6 (5%)   | 1           | 15  |
| 59  | O     | 114/143 (80%) | 88 (77%)   | 24 (21%) | 2 (2%)   | 6           | 34  |
| 60  | DA    | 148/151 (98%) | 146 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 60  | P     | 146/151 (97%) | 144 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 61  | DB    | 120/132 (91%) | 114 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 61  | Q     | 125/132 (95%) | 121 (97%)  | 3 (2%)   | 1 (1%)   | 16          | 49  |
| 62  | DC    | 128/142 (90%) | 97 (76%)   | 27 (21%) | 4 (3%)   | 3           | 25  |
| 62  | R     | 129/142 (91%) | 110 (85%)  | 17 (13%) | 2 (2%)   | 7           | 36  |
| 63  | DD    | 137/142 (96%) | 133 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 63  | S     | 137/142 (96%) | 130 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 64  | DE    | 122/137 (89%) | 119 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 64  | T     | 122/137 (89%) | 118 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 65  | DF    | 139/145 (96%) | 133 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 65  | U     | 142/145 (98%) | 137 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 66  | DG    | 139/145 (96%) | 134 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 66  | V     | 139/145 (96%) | 136 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 67  | DH    | 95/119 (80%)  | 93 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 67  | W     | 100/119 (84%) | 97 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 68  | DI    | 85/87 (98%)   | 83 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 68  | X     | 85/87 (98%)   | 83 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 69  | DJ    | 127/130 (98%) | 124 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 69  | Y     | 127/130 (98%) | 125 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 70  | DK    | 141/145 (97%) | 138 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 70  | Z     | 141/145 (97%) | 138 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 71  | DL    | 130/135 (96%) | 130 (100%) | 0        | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 71  | a     | 132/135 (98%)     | 129 (98%)   | 3 (2%)    | 0        | 100         | 100 |
| 72  | DM    | 69/105 (66%)      | 66 (96%)    | 3 (4%)    | 0        | 100         | 100 |
| 72  | b     | 70/105 (67%)      | 69 (99%)    | 1 (1%)    | 0        | 100         | 100 |
| 73  | DN    | 96/119 (81%)      | 94 (98%)    | 2 (2%)    | 0        | 100         | 100 |
| 73  | c     | 95/119 (80%)      | 93 (98%)    | 2 (2%)    | 0        | 100         | 100 |
| 74  | DO    | 79/82 (96%)       | 72 (91%)    | 7 (9%)    | 0        | 100         | 100 |
| 74  | d     | 79/82 (96%)       | 75 (95%)    | 4 (5%)    | 0        | 100         | 100 |
| 75  | DP    | 59/67 (88%)       | 54 (92%)    | 5 (8%)    | 0        | 100         | 100 |
| 75  | e     | 58/67 (87%)       | 55 (95%)    | 3 (5%)    | 0        | 100         | 100 |
| 76  | DQ    | 52/56 (93%)       | 50 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 76  | f     | 53/56 (95%)       | 51 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 77  | DR    | 57/63 (90%)       | 50 (88%)    | 6 (10%)   | 1 (2%)   | 6           | 34  |
| 77  | g     | 58/63 (92%)       | 53 (91%)    | 5 (9%)    | 0        | 100         | 100 |
| 78  | DS    | 64/193 (33%)      | 31 (48%)    | 23 (36%)  | 10 (16%) | 0           | 2   |
| 78  | h     | 68/193 (35%)      | 56 (82%)    | 11 (16%)  | 1 (2%)   | 8           | 37  |
| 79  | AR    | 309/317 (98%)     | 291 (94%)   | 17 (6%)   | 1 (0%)   | 36          | 67  |
| 79  | DT    | 303/317 (96%)     | 221 (73%)   | 65 (22%)  | 17 (6%)  | 1           | 13  |
| 80  | BE    | 201/220 (91%)     | 197 (98%)   | 4 (2%)    | 0        | 100         | 100 |
| 81  | P0    | 105/312 (34%)     | 69 (66%)    | 27 (26%)  | 9 (9%)   | 0           | 7   |
| 82  | 12    | 61/165 (37%)      | 36 (59%)    | 22 (36%)  | 3 (5%)   | 1           | 16  |
| All | All   | 22176/24752 (90%) | 21009 (95%) | 1028 (5%) | 139 (1%) | 21          | 54  |

All (139) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | l     | 267 | SER  |
| 10  | p     | 205 | ASN  |
| 45  | i     | 36  | SER  |
| 45  | i     | 37  | LYS  |
| 45  | i     | 44  | ALA  |
| 45  | i     | 50  | LYS  |
| 45  | i     | 52  | LYS  |
| 45  | i     | 66  | ASN  |
| 45  | i     | 72  | ASP  |
| 45  | i     | 76  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | i     | 112 | LYS  |
| 59  | O     | 130 | SER  |
| 61  | Q     | 119 | ASP  |
| 14  | BG    | 17  | HIS  |
| 14  | BG    | 48  | PRO  |
| 14  | BG    | 127 | ASP  |
| 14  | BG    | 154 | PRO  |
| 23  | BP    | 61  | ASP  |
| 28  | BU    | 128 | LYS  |
| 39  | CF    | 72  | THR  |
| 41  | CH    | 4   | PRO  |
| 45  | CL    | 41  | ALA  |
| 45  | CL    | 43  | PRO  |
| 45  | CL    | 48  | PRO  |
| 45  | CL    | 160 | LEU  |
| 48  | CO    | 43  | VAL  |
| 48  | CO    | 59  | ASP  |
| 48  | CO    | 212 | ILE  |
| 52  | CS    | 101 | GLY  |
| 52  | CS    | 206 | SER  |
| 54  | CU    | 83  | ASP  |
| 54  | CU    | 128 | PRO  |
| 59  | CZ    | 69  | GLU  |
| 59  | CZ    | 70  | SER  |
| 59  | CZ    | 117 | GLY  |
| 62  | DC    | 18  | LYS  |
| 62  | DC    | 129 | GLY  |
| 78  | DS    | 162 | GLU  |
| 78  | DS    | 167 | THR  |
| 78  | DS    | 174 | MET  |
| 79  | DT    | 5   | GLU  |
| 79  | DT    | 162 | GLN  |
| 79  | DT    | 265 | ARG  |
| 79  | DT    | 277 | VAL  |
| 81  | P0    | 72  | GLU  |
| 82  | 12    | 160 | ILE  |
| 30  | AC    | 58  | ARG  |
| 45  | i     | 57  | PRO  |
| 45  | i     | 81  | THR  |
| 57  | M     | 88  | PRO  |
| 10  | BC    | 183 | GLY  |
| 10  | BC    | 226 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BP    | 64  | VAL  |
| 28  | BU    | 127 | ASN  |
| 39  | CF    | 71  | PRO  |
| 45  | CL    | 55  | LYS  |
| 45  | CL    | 64  | LEU  |
| 54  | CU    | 100 | ARG  |
| 54  | CU    | 159 | ASP  |
| 59  | CZ    | 81  | GLU  |
| 59  | CZ    | 82  | PRO  |
| 59  | CZ    | 121 | VAL  |
| 62  | DC    | 7   | PRO  |
| 77  | DR    | 33  | ARG  |
| 78  | DS    | 158 | ARG  |
| 78  | DS    | 182 | TYR  |
| 79  | DT    | 21  | THR  |
| 79  | DT    | 102 | GLN  |
| 79  | DT    | 157 | ILE  |
| 79  | DT    | 163 | SER  |
| 79  | DT    | 247 | TYR  |
| 81  | P0    | 3   | GLY  |
| 81  | P0    | 75  | LYS  |
| 81  | P0    | 77  | LEU  |
| 81  | P0    | 101 | VAL  |
| 45  | i     | 51  | ALA  |
| 45  | i     | 114 | GLU  |
| 62  | R     | 7   | PRO  |
| 10  | BC    | 100 | PRO  |
| 23  | BP    | 25  | ASN  |
| 26  | BS    | 117 | ASN  |
| 52  | CS    | 153 | GLY  |
| 79  | DT    | 31  | ASP  |
| 79  | DT    | 241 | ALA  |
| 79  | DT    | 263 | GLN  |
| 81  | P0    | 100 | VAL  |
| 23  | 5     | 20  | ALA  |
| 9   | BB    | 230 | GLU  |
| 10  | BC    | 127 | SER  |
| 14  | BG    | 166 | GLN  |
| 23  | BP    | 24  | GLU  |
| 32  | BY    | 83  | ASP  |
| 39  | CF    | 21  | LYS  |
| 45  | CL    | 46  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | CL    | 56  | SER  |
| 45  | CL    | 62  | ALA  |
| 48  | CO    | 29  | TRP  |
| 48  | CO    | 80  | SER  |
| 79  | DT    | 160 | SER  |
| 79  | DT    | 296 | GLN  |
| 81  | P0    | 107 | ALA  |
| 23  | 5     | 11  | SER  |
| 45  | i     | 47  | ASP  |
| 57  | M     | 92  | LEU  |
| 59  | O     | 104 | CYS  |
| 14  | BG    | 164 | PRO  |
| 23  | BP    | 13  | LYS  |
| 25  | BR    | 97  | LYS  |
| 48  | CO    | 51  | SER  |
| 54  | CU    | 51  | LYS  |
| 62  | DC    | 16  | SER  |
| 78  | DS    | 142 | LEU  |
| 78  | DS    | 143 | ALA  |
| 78  | DS    | 164 | PRO  |
| 78  | DS    | 179 | ASP  |
| 79  | DT    | 262 | LEU  |
| 82  | 12    | 105 | PRO  |
| 82  | 12    | 106 | LEU  |
| 5   | k     | 139 | THR  |
| 30  | AC    | 3   | LYS  |
| 45  | i     | 61  | GLU  |
| 45  | i     | 65  | LYS  |
| 45  | i     | 69  | PHE  |
| 78  | h     | 141 | LYS  |
| 79  | AR    | 203 | PRO  |
| 10  | BC    | 128 | PRO  |
| 14  | BG    | 49  | ARG  |
| 45  | CL    | 88  | PHE  |
| 54  | CU    | 82  | PRO  |
| 79  | DT    | 74  | ILE  |
| 79  | DT    | 95  | LEU  |
| 45  | i     | 73  | VAL  |
| 23  | BP    | 68  | VAL  |
| 36  | CC    | 39  | PRO  |
| 81  | P0    | 28  | VAL  |
| 30  | AC    | 21  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | R     | 2   | VAL  |
| 81  | P0    | 25  | ILE  |
| 78  | DS    | 129 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 4   | AW    | 190/194 (98%) | 190 (100%) | 0        | 100         | 100 |
| 4   | j     | 190/194 (98%) | 190 (100%) | 0        | 100         | 100 |
| 5   | AX    | 325/328 (99%) | 325 (100%) | 0        | 100         | 100 |
| 5   | k     | 325/328 (99%) | 325 (100%) | 0        | 100         | 100 |
| 6   | AY    | 288/292 (99%) | 288 (100%) | 0        | 100         | 100 |
| 6   | l     | 288/292 (99%) | 288 (100%) | 0        | 100         | 100 |
| 7   | AZ    | 247/252 (98%) | 247 (100%) | 0        | 100         | 100 |
| 7   | m     | 248/252 (98%) | 248 (100%) | 0        | 100         | 100 |
| 8   | BA    | 132/154 (86%) | 132 (100%) | 0        | 100         | 100 |
| 8   | n     | 136/154 (88%) | 136 (100%) | 0        | 100         | 100 |
| 9   | BB    | 190/204 (93%) | 190 (100%) | 0        | 100         | 100 |
| 9   | o     | 193/204 (95%) | 193 (100%) | 0        | 100         | 100 |
| 10  | BC    | 193/216 (89%) | 191 (99%)  | 2 (1%)   | 68          | 75  |
| 10  | p     | 196/216 (91%) | 196 (100%) | 0        | 100         | 100 |
| 11  | BD    | 169/170 (99%) | 169 (100%) | 0        | 100         | 100 |
| 11  | q     | 169/170 (99%) | 169 (100%) | 0        | 100         | 100 |
| 12  | r     | 177/185 (96%) | 177 (100%) | 0        | 100         | 100 |
| 13  | BF    | 146/149 (98%) | 146 (100%) | 0        | 100         | 100 |
| 13  | s     | 146/149 (98%) | 146 (100%) | 0        | 100         | 100 |
| 14  | BG    | 166/168 (99%) | 164 (99%)  | 2 (1%)   | 63          | 73  |
| 14  | t     | 166/168 (99%) | 166 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 15  | BH    | 108/109 (99%) | 108 (100%) | 0        | 100         | 100 |
| 15  | u     | 107/109 (98%) | 107 (100%) | 0        | 100         | 100 |
| 16  | BI    | 177/178 (99%) | 177 (100%) | 0        | 100         | 100 |
| 16  | v     | 177/178 (99%) | 177 (100%) | 0        | 100         | 100 |
| 17  | BJ    | 166/167 (99%) | 166 (100%) | 0        | 100         | 100 |
| 17  | w     | 166/167 (99%) | 166 (100%) | 0        | 100         | 100 |
| 18  | BK    | 145/154 (94%) | 145 (100%) | 0        | 100         | 100 |
| 18  | x     | 140/154 (91%) | 139 (99%)  | 1 (1%)   | 76          | 78  |
| 19  | BL    | 153/154 (99%) | 153 (100%) | 0        | 100         | 100 |
| 19  | y     | 153/154 (99%) | 153 (100%) | 0        | 100         | 100 |
| 20  | BM    | 146/153 (95%) | 144 (99%)  | 2 (1%)   | 59          | 71  |
| 20  | z     | 146/153 (95%) | 144 (99%)  | 2 (1%)   | 59          | 71  |
| 21  | 0     | 155/157 (99%) | 155 (100%) | 0        | 100         | 100 |
| 21  | BN    | 155/157 (99%) | 154 (99%)  | 1 (1%)   | 78          | 79  |
| 22  | 2     | 133/134 (99%) | 133 (100%) | 0        | 100         | 100 |
| 22  | BO    | 133/134 (99%) | 133 (100%) | 0        | 100         | 100 |
| 23  | 5     | 91/112 (81%)  | 89 (98%)   | 2 (2%)   | 45          | 65  |
| 23  | BP    | 90/112 (80%)  | 90 (100%)  | 0        | 100         | 100 |
| 24  | 6     | 101/104 (97%) | 101 (100%) | 0        | 100         | 100 |
| 24  | BQ    | 101/104 (97%) | 101 (100%) | 0        | 100         | 100 |
| 25  | 7     | 97/127 (76%)  | 94 (97%)   | 3 (3%)   | 35          | 59  |
| 25  | BR    | 91/127 (72%)  | 91 (100%)  | 0        | 100         | 100 |
| 26  | 8     | 107/121 (88%) | 107 (100%) | 0        | 100         | 100 |
| 26  | BS    | 107/121 (88%) | 107 (100%) | 0        | 100         | 100 |
| 27  | 9     | 111/112 (99%) | 111 (100%) | 0        | 100         | 100 |
| 27  | BT    | 111/112 (99%) | 111 (100%) | 0        | 100         | 100 |
| 28  | AA    | 117/118 (99%) | 117 (100%) | 0        | 100         | 100 |
| 28  | BU    | 117/118 (99%) | 117 (100%) | 0        | 100         | 100 |
| 29  | AB    | 120/121 (99%) | 120 (100%) | 0        | 100         | 100 |
| 29  | BV    | 120/121 (99%) | 120 (100%) | 0        | 100         | 100 |
| 30  | AC    | 45/49 (92%)   | 45 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 30  | BW    | 47/49 (96%)   | 47 (100%)  | 0        | 100         | 100 |
| 31  | AD    | 83/90 (92%)   | 80 (96%)   | 3 (4%)   | 31          | 57  |
| 31  | BX    | 79/90 (88%)   | 79 (100%)  | 0        | 100         | 100 |
| 32  | AE    | 97/100 (97%)  | 97 (100%)  | 0        | 100         | 100 |
| 32  | BY    | 97/100 (97%)  | 97 (100%)  | 0        | 100         | 100 |
| 33  | AF    | 109/115 (95%) | 109 (100%) | 0        | 100         | 100 |
| 33  | BZ    | 109/115 (95%) | 109 (100%) | 0        | 100         | 100 |
| 34  | AG    | 91/92 (99%)   | 91 (100%)  | 0        | 100         | 100 |
| 34  | CA    | 91/92 (99%)   | 91 (100%)  | 0        | 100         | 100 |
| 35  | AH    | 95/102 (93%)  | 95 (100%)  | 0        | 100         | 100 |
| 35  | CB    | 93/102 (91%)  | 93 (100%)  | 0        | 100         | 100 |
| 36  | AI    | 104/106 (98%) | 104 (100%) | 0        | 100         | 100 |
| 36  | CC    | 105/106 (99%) | 103 (98%)  | 2 (2%)   | 50          | 68  |
| 37  | AJ    | 77/79 (98%)   | 77 (100%)  | 0        | 100         | 100 |
| 37  | CD    | 75/79 (95%)   | 74 (99%)   | 1 (1%)   | 61          | 72  |
| 38  | AK    | 70/73 (96%)   | 70 (100%)  | 0        | 100         | 100 |
| 38  | CE    | 70/73 (96%)   | 70 (100%)  | 0        | 100         | 100 |
| 39  | AL    | 68/69 (99%)   | 68 (100%)  | 0        | 100         | 100 |
| 39  | CF    | 68/69 (99%)   | 68 (100%)  | 0        | 100         | 100 |
| 40  | AM    | 46/47 (98%)   | 46 (100%)  | 0        | 100         | 100 |
| 40  | CG    | 46/47 (98%)   | 46 (100%)  | 0        | 100         | 100 |
| 41  | AN    | 45/47 (96%)   | 45 (100%)  | 0        | 100         | 100 |
| 41  | CH    | 45/47 (96%)   | 45 (100%)  | 0        | 100         | 100 |
| 42  | AO    | 24/24 (100%)  | 24 (100%)  | 0        | 100         | 100 |
| 42  | CI    | 23/24 (96%)   | 23 (100%)  | 0        | 100         | 100 |
| 43  | AP    | 88/91 (97%)   | 88 (100%)  | 0        | 100         | 100 |
| 43  | CJ    | 88/91 (97%)   | 88 (100%)  | 0        | 100         | 100 |
| 44  | AQ    | 72/73 (99%)   | 72 (100%)  | 0        | 100         | 100 |
| 44  | CK    | 72/73 (99%)   | 72 (100%)  | 0        | 100         | 100 |
| 45  | CL    | 99/212 (47%)  | 97 (98%)   | 2 (2%)   | 48          | 67  |
| 45  | i     | 86/212 (41%)  | 83 (96%)   | 3 (4%)   | 32          | 57  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 47  | C     | 176/215 (82%)  | 176 (100%) | 0        | 100         | 100 |
| 47  | CN    | 176/215 (82%)  | 176 (100%) | 0        | 100         | 100 |
| 48  | CO    | 193/229 (84%)  | 192 (100%) | 1 (0%)   | 81          | 80  |
| 48  | D     | 194/229 (85%)  | 194 (100%) | 0        | 100         | 100 |
| 49  | CP    | 175/198 (88%)  | 175 (100%) | 0        | 100         | 100 |
| 49  | E     | 175/198 (88%)  | 175 (100%) | 0        | 100         | 100 |
| 50  | CQ    | 174/196 (89%)  | 174 (100%) | 0        | 100         | 100 |
| 50  | F     | 174/196 (89%)  | 174 (100%) | 0        | 100         | 100 |
| 51  | CR    | 218/220 (99%)  | 218 (100%) | 0        | 100         | 100 |
| 51  | G     | 217/220 (99%)  | 217 (100%) | 0        | 100         | 100 |
| 52  | CS    | 177/197 (90%)  | 172 (97%)  | 5 (3%)   | 38          | 61  |
| 52  | H     | 178/197 (90%)  | 178 (100%) | 0        | 100         | 100 |
| 53  | CT    | 204/204 (100%) | 204 (100%) | 0        | 100         | 100 |
| 53  | I     | 193/204 (95%)  | 193 (100%) | 0        | 100         | 100 |
| 54  | CU    | 161/167 (96%)  | 161 (100%) | 0        | 100         | 100 |
| 54  | J     | 163/167 (98%)  | 163 (100%) | 0        | 100         | 100 |
| 55  | CV    | 157/160 (98%)  | 157 (100%) | 0        | 100         | 100 |
| 55  | K     | 157/160 (98%)  | 157 (100%) | 0        | 100         | 100 |
| 56  | CW    | 153/160 (96%)  | 153 (100%) | 0        | 100         | 100 |
| 56  | L     | 153/160 (96%)  | 153 (100%) | 0        | 100         | 100 |
| 57  | CX    | 88/104 (85%)   | 88 (100%)  | 0        | 100         | 100 |
| 57  | M     | 90/104 (86%)   | 89 (99%)   | 1 (1%)   | 65          | 74  |
| 58  | CY    | 122/134 (91%)  | 121 (99%)  | 1 (1%)   | 73          | 77  |
| 58  | N     | 124/134 (92%)  | 124 (100%) | 0        | 100         | 100 |
| 59  | CZ    | 101/123 (82%)  | 101 (100%) | 0        | 100         | 100 |
| 59  | O     | 98/123 (80%)   | 94 (96%)   | 4 (4%)   | 27          | 53  |
| 60  | DA    | 129/130 (99%)  | 129 (100%) | 0        | 100         | 100 |
| 60  | P     | 128/130 (98%)  | 128 (100%) | 0        | 100         | 100 |
| 61  | DB    | 93/102 (91%)   | 93 (100%)  | 0        | 100         | 100 |
| 61  | Q     | 97/102 (95%)   | 97 (100%)  | 0        | 100         | 100 |
| 62  | DC    | 112/121 (93%)  | 112 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 62  | R     | 112/121 (93%) | 112 (100%) | 0        | 100         | 100 |
| 63  | DD    | 113/116 (97%) | 113 (100%) | 0        | 100         | 100 |
| 63  | S     | 113/116 (97%) | 111 (98%)  | 2 (2%)   | 51          | 69  |
| 64  | DE    | 112/122 (92%) | 112 (100%) | 0        | 100         | 100 |
| 64  | T     | 112/122 (92%) | 112 (100%) | 0        | 100         | 100 |
| 65  | DF    | 125/129 (97%) | 123 (98%)  | 2 (2%)   | 55          | 70  |
| 65  | U     | 128/129 (99%) | 127 (99%)  | 1 (1%)   | 73          | 77  |
| 66  | DG    | 113/117 (97%) | 113 (100%) | 0        | 100         | 100 |
| 66  | V     | 113/117 (97%) | 113 (100%) | 0        | 100         | 100 |
| 67  | DH    | 87/105 (83%)  | 87 (100%)  | 0        | 100         | 100 |
| 67  | W     | 92/105 (88%)  | 92 (100%)  | 0        | 100         | 100 |
| 68  | DI    | 71/71 (100%)  | 71 (100%)  | 0        | 100         | 100 |
| 68  | X     | 71/71 (100%)  | 71 (100%)  | 0        | 100         | 100 |
| 69  | DJ    | 112/113 (99%) | 112 (100%) | 0        | 100         | 100 |
| 69  | Y     | 112/113 (99%) | 112 (100%) | 0        | 100         | 100 |
| 70  | DK    | 116/118 (98%) | 116 (100%) | 0        | 100         | 100 |
| 70  | Z     | 116/118 (98%) | 116 (100%) | 0        | 100         | 100 |
| 71  | DL    | 109/112 (97%) | 109 (100%) | 0        | 100         | 100 |
| 71  | a     | 111/112 (99%) | 111 (100%) | 0        | 100         | 100 |
| 72  | DM    | 63/85 (74%)   | 63 (100%)  | 0        | 100         | 100 |
| 72  | b     | 64/85 (75%)   | 64 (100%)  | 0        | 100         | 100 |
| 73  | DN    | 84/102 (82%)  | 84 (100%)  | 0        | 100         | 100 |
| 73  | c     | 83/102 (81%)  | 83 (100%)  | 0        | 100         | 100 |
| 74  | DO    | 72/73 (99%)   | 72 (100%)  | 0        | 100         | 100 |
| 74  | d     | 72/73 (99%)   | 72 (100%)  | 0        | 100         | 100 |
| 75  | DP    | 53/58 (91%)   | 53 (100%)  | 0        | 100         | 100 |
| 75  | e     | 52/58 (90%)   | 52 (100%)  | 0        | 100         | 100 |
| 76  | DQ    | 47/48 (98%)   | 46 (98%)   | 1 (2%)   | 47          | 66  |
| 76  | f     | 47/48 (98%)   | 43 (92%)   | 4 (8%)   | 10          | 34  |
| 77  | DR    | 51/54 (94%)   | 49 (96%)   | 2 (4%)   | 28          | 54  |
| 77  | g     | 51/54 (94%)   | 51 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 78  | DS    | 60/175 (34%)      | 59 (98%)     | 1 (2%)   | 53          | 70  |
| 78  | h     | 62/175 (35%)      | 61 (98%)     | 1 (2%)   | 55          | 70  |
| 79  | AR    | 259/263 (98%)     | 259 (100%)   | 0        | 100         | 100 |
| 79  | DT    | 255/263 (97%)     | 248 (97%)    | 7 (3%)   | 39          | 62  |
| 80  | BE    | 175/186 (94%)     | 175 (100%)   | 0        | 100         | 100 |
| 81  | P0    | 92/247 (37%)      | 92 (100%)    | 0        | 100         | 100 |
| 82  | 12    | 53/137 (39%)      | 50 (94%)     | 3 (6%)   | 18          | 45  |
| All | All   | 19011/20831 (91%) | 18949 (100%) | 62 (0%)  | 86          | 83  |

All (62) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | x     | 180 | LYS  |
| 20  | z     | 162 | ARG  |
| 20  | z     | 165 | ARG  |
| 23  | 5     | 13  | LYS  |
| 23  | 5     | 14  | LYS  |
| 25  | 7     | 113 | LYS  |
| 25  | 7     | 116 | LYS  |
| 25  | 7     | 117 | LYS  |
| 31  | AD    | 9   | GLN  |
| 31  | AD    | 10  | GLU  |
| 31  | AD    | 11  | ASN  |
| 45  | i     | 115 | LEU  |
| 45  | i     | 137 | ASP  |
| 45  | i     | 138 | GLU  |
| 57  | M     | 8   | ARG  |
| 59  | O     | 36  | LEU  |
| 59  | O     | 38  | HIS  |
| 59  | O     | 39  | ASP  |
| 59  | O     | 41  | LEU  |
| 63  | S     | 38  | VAL  |
| 63  | S     | 39  | GLN  |
| 65  | U     | 138 | THR  |
| 76  | f     | 24  | CYS  |
| 76  | f     | 36  | LEU  |
| 76  | f     | 38  | LEU  |
| 76  | f     | 39  | CYS  |
| 78  | h     | 168 | CYS  |
| 10  | BC    | 182 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | BC    | 224 | ILE  |
| 14  | BG    | 46  | ILE  |
| 14  | BG    | 48  | PRO  |
| 20  | BM    | 130 | ASN  |
| 20  | BM    | 174 | GLN  |
| 21  | BN    | 13  | ASN  |
| 36  | CC    | 38  | ARG  |
| 36  | CC    | 40  | SER  |
| 37  | CD    | 87  | GLU  |
| 45  | CL    | 47  | ASP  |
| 45  | CL    | 99  | SER  |
| 48  | CO    | 85  | LYS  |
| 52  | CS    | 22  | VAL  |
| 52  | CS    | 23  | VAL  |
| 52  | CS    | 86  | GLN  |
| 52  | CS    | 180 | ARG  |
| 52  | CS    | 183 | SER  |
| 58  | CY    | 46  | LYS  |
| 65  | DF    | 25  | ARG  |
| 65  | DF    | 138 | THR  |
| 76  | DQ    | 42  | CYS  |
| 77  | DR    | 29  | LYS  |
| 77  | DR    | 31  | GLN  |
| 78  | DS    | 163 | CYS  |
| 79  | DT    | 20  | VAL  |
| 79  | DT    | 22  | SER  |
| 79  | DT    | 65  | HIS  |
| 79  | DT    | 66  | SER  |
| 79  | DT    | 92  | LEU  |
| 79  | DT    | 93  | TRP  |
| 79  | DT    | 160 | SER  |
| 82  | 12    | 103 | ASN  |
| 82  | 12    | 104 | ILE  |
| 82  | 12    | 106 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | k     | 182 | GLN  |
| 5   | k     | 198 | HIS  |
| 5   | k     | 259 | ASN  |
| 5   | k     | 316 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | l     | 56  | ASN  |
| 6   | l     | 214 | ASN  |
| 6   | l     | 284 | ASN  |
| 6   | l     | 308 | GLN  |
| 6   | l     | 312 | HIS  |
| 6   | l     | 356 | GLN  |
| 7   | m     | 13  | HIS  |
| 7   | m     | 17  | GLN  |
| 7   | m     | 94  | ASN  |
| 7   | m     | 244 | HIS  |
| 9   | o     | 17  | GLN  |
| 9   | o     | 78  | GLN  |
| 9   | o     | 91  | ASN  |
| 9   | o     | 144 | GLN  |
| 9   | o     | 198 | ASN  |
| 9   | o     | 228 | ASN  |
| 11  | q     | 5   | GLN  |
| 11  | q     | 116 | ASN  |
| 11  | q     | 157 | ASN  |
| 12  | r     | 100 | ASN  |
| 13  | s     | 161 | GLN  |
| 15  | u     | 35  | GLN  |
| 15  | u     | 112 | GLN  |
| 16  | v     | 15  | GLN  |
| 16  | v     | 86  | ASN  |
| 16  | v     | 123 | GLN  |
| 17  | w     | 51  | ASN  |
| 17  | w     | 56  | HIS  |
| 17  | w     | 164 | GLN  |
| 18  | x     | 97  | ASN  |
| 18  | x     | 125 | GLN  |
| 19  | y     | 9   | GLN  |
| 19  | y     | 58  | ASN  |
| 21  | 0     | 62  | ASN  |
| 25  | 7     | 79  | GLN  |
| 29  | AB    | 40  | HIS  |
| 29  | AB    | 65  | GLN  |
| 30  | AC    | 12  | GLN  |
| 31  | AD    | 11  | ASN  |
| 31  | AD    | 73  | GLN  |
| 34  | AG    | 75  | HIS  |
| 36  | AI    | 107 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | AI    | 113 | GLN  |
| 38  | AK    | 69  | HIS  |
| 39  | AL    | 40  | GLN  |
| 39  | AL    | 51  | GLN  |
| 39  | AL    | 57  | ASN  |
| 39  | AL    | 67  | GLN  |
| 40  | AM    | 33  | ASN  |
| 43  | AP    | 23  | HIS  |
| 44  | AQ    | 48  | GLN  |
| 45  | i     | 109 | GLN  |
| 47  | C     | 21  | ASN  |
| 47  | C     | 30  | GLN  |
| 47  | C     | 33  | ASN  |
| 47  | C     | 49  | ASN  |
| 49  | E     | 84  | GLN  |
| 49  | E     | 204 | ASN  |
| 50  | F     | 57  | GLN  |
| 51  | G     | 68  | GLN  |
| 51  | G     | 188 | ASN  |
| 53  | I     | 22  | HIS  |
| 53  | I     | 199 | GLN  |
| 54  | J     | 19  | GLN  |
| 54  | J     | 38  | GLN  |
| 55  | K     | 103 | GLN  |
| 55  | K     | 116 | HIS  |
| 57  | M     | 39  | ASN  |
| 57  | M     | 62  | GLN  |
| 59  | O     | 134 | ASN  |
| 60  | P     | 5   | HIS  |
| 60  | P     | 105 | ASN  |
| 62  | R     | 79  | HIS  |
| 63  | S     | 39  | GLN  |
| 65  | U     | 19  | ASN  |
| 65  | U     | 75  | ASN  |
| 66  | V     | 85  | ASN  |
| 67  | W     | 35  | ASN  |
| 68  | X     | 21  | ASN  |
| 69  | Y     | 70  | ASN  |
| 70  | Z     | 94  | ASN  |
| 71  | a     | 22  | GLN  |
| 71  | a     | 106 | GLN  |
| 72  | b     | 37  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 73  | c     | 25  | ASN  |
| 79  | AR    | 16  | HIS  |
| 79  | AR    | 102 | GLN  |
| 4   | AW    | 86  | GLN  |
| 5   | AX    | 182 | GLN  |
| 5   | AX    | 198 | HIS  |
| 5   | AX    | 259 | ASN  |
| 5   | AX    | 316 | ASN  |
| 6   | AY    | 6   | GLN  |
| 6   | AY    | 16  | GLN  |
| 6   | AY    | 46  | ASN  |
| 6   | AY    | 111 | ASN  |
| 6   | AY    | 117 | ASN  |
| 6   | AY    | 222 | ASN  |
| 6   | AY    | 321 | ASN  |
| 6   | AY    | 329 | ASN  |
| 6   | AY    | 356 | GLN  |
| 8   | BA    | 172 | HIS  |
| 9   | BB    | 50  | GLN  |
| 9   | BB    | 144 | GLN  |
| 9   | BB    | 198 | ASN  |
| 9   | BB    | 218 | GLN  |
| 10  | BC    | 39  | GLN  |
| 10  | BC    | 62  | GLN  |
| 10  | BC    | 139 | HIS  |
| 10  | BC    | 156 | ASN  |
| 10  | BC    | 205 | ASN  |
| 10  | BC    | 244 | ASN  |
| 11  | BD    | 129 | HIS  |
| 80  | BE    | 162 | GLN  |
| 80  | BE    | 187 | ASN  |
| 13  | BF    | 47  | GLN  |
| 13  | BF    | 109 | HIS  |
| 13  | BF    | 161 | GLN  |
| 14  | BG    | 12  | ASN  |
| 14  | BG    | 99  | HIS  |
| 16  | BI    | 15  | GLN  |
| 16  | BI    | 86  | ASN  |
| 16  | BI    | 194 | HIS  |
| 17  | BJ    | 51  | ASN  |
| 18  | BK    | 97  | ASN  |
| 18  | BK    | 169 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | BM    | 130 | ASN  |
| 20  | BM    | 134 | HIS  |
| 20  | BM    | 175 | GLN  |
| 22  | BO    | 58  | HIS  |
| 22  | BO    | 95  | HIS  |
| 22  | BO    | 112 | ASN  |
| 22  | BO    | 131 | GLN  |
| 23  | BP    | 30  | GLN  |
| 23  | BP    | 71  | ASN  |
| 25  | BR    | 42  | GLN  |
| 26  | BS    | 47  | GLN  |
| 27  | BT    | 81  | GLN  |
| 27  | BT    | 86  | GLN  |
| 28  | BU    | 122 | HIS  |
| 30  | BW    | 6   | ASN  |
| 30  | BW    | 48  | HIS  |
| 31  | BX    | 73  | GLN  |
| 34  | CA    | 24  | ASN  |
| 34  | CA    | 106 | ASN  |
| 37  | CD    | 11  | ASN  |
| 38  | CE    | 20  | ASN  |
| 38  | CE    | 69  | HIS  |
| 38  | CE    | 76  | ASN  |
| 41  | CH    | 44  | GLN  |
| 43  | CJ    | 22  | GLN  |
| 45  | CL    | 83  | HIS  |
| 45  | CL    | 104 | GLN  |
| 47  | CN    | 140 | ASN  |
| 48  | CO    | 40  | ASN  |
| 48  | CO    | 79  | HIS  |
| 48  | CO    | 99  | ASN  |
| 48  | CO    | 146 | GLN  |
| 48  | CO    | 157 | GLN  |
| 48  | CO    | 220 | GLN  |
| 49  | CP    | 84  | GLN  |
| 50  | CQ    | 33  | GLN  |
| 51  | CR    | 17  | HIS  |
| 51  | CR    | 68  | GLN  |
| 51  | CR    | 98  | HIS  |
| 52  | CS    | 37  | GLN  |
| 52  | CS    | 100 | ASN  |
| 52  | CS    | 103 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | CS    | 169 | ASN  |
| 53  | CT    | 182 | GLN  |
| 53  | CT    | 200 | GLN  |
| 55  | CV    | 35  | ASN  |
| 55  | CV    | 116 | HIS  |
| 57  | CX    | 29  | GLN  |
| 57  | CX    | 58  | GLN  |
| 57  | CX    | 81  | ASN  |
| 58  | CY    | 92  | HIS  |
| 59  | CZ    | 134 | ASN  |
| 63  | DD    | 82  | GLN  |
| 63  | DD    | 138 | GLN  |
| 64  | DE    | 42  | GLN  |
| 69  | DJ    | 44  | HIS  |
| 69  | DJ    | 56  | HIS  |
| 69  | DJ    | 64  | GLN  |
| 69  | DJ    | 92  | ASN  |
| 72  | DM    | 38  | HIS  |
| 74  | DO    | 9   | HIS  |
| 76  | DQ    | 53  | ASN  |
| 77  | DR    | 31  | GLN  |
| 78  | DS    | 155 | ASN  |
| 79  | DT    | 16  | HIS  |
| 79  | DT    | 29  | HIS  |
| 79  | DT    | 107 | HIS  |
| 79  | DT    | 225 | ASN  |
| 79  | DT    | 296 | GLN  |
| 81  | P0    | 10  | GLN  |
| 82  | 12    | 103 | ASN  |
| 82  | 12    | 117 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1     | 3215/3359 (95%) | 607 (18%)         | 45 (1%)         |
| 1   | AS    | 3093/3359 (92%) | 528 (17%)         | 39 (1%)         |
| 2   | 3     | 120/121 (99%)   | 9 (7%)            | 0               |
| 2   | AT    | 120/121 (99%)   | 9 (7%)            | 0               |
| 3   | 4     | 155/158 (98%)   | 22 (14%)          | 2 (1%)          |
| 3   | AU    | 157/158 (99%)   | 23 (14%)          | 3 (1%)          |
| 46  | B     | 1702/1787 (95%) | 405 (23%)         | 45 (2%)         |

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| Mol | Chain | Analysed          | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 46  | CM    | 1722/1787 (96%)   | 430 (24%)         | 48 (2%)         |
| All | All   | 10284/10850 (94%) | 2033 (19%)        | 182 (1%)        |

All (2033) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 15  | A    |
| 1   | 1     | 24  | U    |
| 1   | 1     | 25  | A    |
| 1   | 1     | 29  | G    |
| 1   | 1     | 39  | A    |
| 1   | 1     | 42  | A    |
| 1   | 1     | 48  | A    |
| 1   | 1     | 56  | A    |
| 1   | 1     | 58  | G    |
| 1   | 1     | 59  | A    |
| 1   | 1     | 64  | A    |
| 1   | 1     | 65  | A    |
| 1   | 1     | 91  | G    |
| 1   | 1     | 98  | A    |
| 1   | 1     | 104 | C    |
| 1   | 1     | 108 | A    |
| 1   | 1     | 109 | G    |
| 1   | 1     | 110 | C    |
| 1   | 1     | 121 | A    |
| 1   | 1     | 134 | U    |
| 1   | 1     | 135 | G    |
| 1   | 1     | 155 | A    |
| 1   | 1     | 156 | A    |
| 1   | 1     | 164 | U    |
| 1   | 1     | 169 | G    |
| 1   | 1     | 172 | C    |
| 1   | 1     | 173 | C    |
| 1   | 1     | 175 | G    |
| 1   | 1     | 186 | A    |
| 1   | 1     | 189 | U    |
| 1   | 1     | 190 | U    |
| 1   | 1     | 199 | C    |
| 1   | 1     | 205 | G    |
| 1   | 1     | 209 | C    |
| 1   | 1     | 212 | A    |
| 1   | 1     | 217 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 218 | A    |
| 1   | 1     | 219 | G    |
| 1   | 1     | 230 | G    |
| 1   | 1     | 236 | A    |
| 1   | 1     | 239 | A    |
| 1   | 1     | 240 | C    |
| 1   | 1     | 243 | G    |
| 1   | 1     | 245 | G    |
| 1   | 1     | 249 | G    |
| 1   | 1     | 250 | U    |
| 1   | 1     | 269 | G    |
| 1   | 1     | 286 | U    |
| 1   | 1     | 295 | A    |
| 1   | 1     | 305 | U    |
| 1   | 1     | 311 | C    |
| 1   | 1     | 323 | A    |
| 1   | 1     | 329 | U    |
| 1   | 1     | 337 | G    |
| 1   | 1     | 338 | A    |
| 1   | 1     | 339 | C    |
| 1   | 1     | 349 | A    |
| 1   | 1     | 350 | C    |
| 1   | 1     | 376 | G    |
| 1   | 1     | 377 | A    |
| 1   | 1     | 387 | A    |
| 1   | 1     | 395 | A    |
| 1   | 1     | 398 | A    |
| 1   | 1     | 402 | A    |
| 1   | 1     | 403 | C    |
| 1   | 1     | 404 | G    |
| 1   | 1     | 420 | G    |
| 1   | 1     | 421 | G    |
| 1   | 1     | 422 | A    |
| 1   | 1     | 438 | A    |
| 1   | 1     | 439 | C    |
| 1   | 1     | 448 | U    |
| 1   | 1     | 450 | G    |
| 1   | 1     | 451 | C    |
| 1   | 1     | 481 | G    |
| 1   | 1     | 482 | U    |
| 1   | 1     | 506 | A    |
| 1   | 1     | 517 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 519 | U    |
| 1   | 1     | 531 | G    |
| 1   | 1     | 532 | U    |
| 1   | 1     | 538 | G    |
| 1   | 1     | 539 | G    |
| 1   | 1     | 540 | C    |
| 1   | 1     | 541 | U    |
| 1   | 1     | 542 | U    |
| 1   | 1     | 543 | C    |
| 1   | 1     | 544 | U    |
| 1   | 1     | 545 | G    |
| 1   | 1     | 546 | C    |
| 1   | 1     | 555 | A    |
| 1   | 1     | 556 | U    |
| 1   | 1     | 557 | A    |
| 1   | 1     | 564 | G    |
| 1   | 1     | 577 | G    |
| 1   | 1     | 589 | G    |
| 1   | 1     | 590 | A    |
| 1   | 1     | 598 | U    |
| 1   | 1     | 600 | U    |
| 1   | 1     | 601 | U    |
| 1   | 1     | 602 | A    |
| 1   | 1     | 609 | A    |
| 1   | 1     | 618 | U    |
| 1   | 1     | 619 | A    |
| 1   | 1     | 620 | A    |
| 1   | 1     | 635 | C    |
| 1   | 1     | 647 | A    |
| 1   | 1     | 658 | A    |
| 1   | 1     | 675 | A    |
| 1   | 1     | 679 | U    |
| 1   | 1     | 681 | U    |
| 1   | 1     | 688 | A    |
| 1   | 1     | 689 | A    |
| 1   | 1     | 703 | A    |
| 1   | 1     | 710 | G    |
| 1   | 1     | 713 | A    |
| 1   | 1     | 717 | A    |
| 1   | 1     | 723 | G    |
| 1   | 1     | 730 | A    |
| 1   | 1     | 732 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 760  | U    |
| 1   | 1     | 763  | U    |
| 1   | 1     | 772  | U    |
| 1   | 1     | 773  | U    |
| 1   | 1     | 776  | A    |
| 1   | 1     | 777  | G    |
| 1   | 1     | 780  | A    |
| 1   | 1     | 781  | G    |
| 1   | 1     | 802  | A    |
| 1   | 1     | 812  | A    |
| 1   | 1     | 813  | A    |
| 1   | 1     | 826  | A    |
| 1   | 1     | 845  | C    |
| 1   | 1     | 857  | C    |
| 1   | 1     | 861  | U    |
| 1   | 1     | 870  | U    |
| 1   | 1     | 875  | U    |
| 1   | 1     | 903  | G    |
| 1   | 1     | 904  | G    |
| 1   | 1     | 910  | A    |
| 1   | 1     | 912  | G    |
| 1   | 1     | 913  | A    |
| 1   | 1     | 917  | A    |
| 1   | 1     | 919  | C    |
| 1   | 1     | 921  | A    |
| 1   | 1     | 933  | G    |
| 1   | 1     | 940  | C    |
| 1   | 1     | 949  | G    |
| 1   | 1     | 955  | C    |
| 1   | 1     | 956  | U    |
| 1   | 1     | 958  | A    |
| 1   | 1     | 959  | G    |
| 1   | 1     | 977  | U    |
| 1   | 1     | 990  | G    |
| 1   | 1     | 991  | U    |
| 1   | 1     | 996  | C    |
| 1   | 1     | 997  | G    |
| 1   | 1     | 998  | A    |
| 1   | 1     | 1006 | G    |
| 1   | 1     | 1011 | C    |
| 1   | 1     | 1012 | U    |
| 1   | 1     | 1013 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1014 | G    |
| 1   | 1     | 1018 | U    |
| 1   | 1     | 1019 | U    |
| 1   | 1     | 1020 | G    |
| 1   | 1     | 1021 | A    |
| 1   | 1     | 1023 | A    |
| 1   | 1     | 1024 | U    |
| 1   | 1     | 1027 | C    |
| 1   | 1     | 1030 | U    |
| 1   | 1     | 1033 | C    |
| 1   | 1     | 1043 | A    |
| 1   | 1     | 1045 | C    |
| 1   | 1     | 1060 | A    |
| 1   | 1     | 1061 | A    |
| 1   | 1     | 1068 | G    |
| 1   | 1     | 1077 | U    |
| 1   | 1     | 1078 | U    |
| 1   | 1     | 1089 | A    |
| 1   | 1     | 1090 | A    |
| 1   | 1     | 1091 | U    |
| 1   | 1     | 1092 | U    |
| 1   | 1     | 1094 | A    |
| 1   | 1     | 1099 | A    |
| 1   | 1     | 1100 | G    |
| 1   | 1     | 1113 | G    |
| 1   | 1     | 1127 | G    |
| 1   | 1     | 1140 | U    |
| 1   | 1     | 1149 | A    |
| 1   | 1     | 1150 | A    |
| 1   | 1     | 1151 | C    |
| 1   | 1     | 1155 | A    |
| 1   | 1     | 1156 | C    |
| 1   | 1     | 1164 | U    |
| 1   | 1     | 1174 | G    |
| 1   | 1     | 1176 | A    |
| 1   | 1     | 1177 | U    |
| 1   | 1     | 1178 | G    |
| 1   | 1     | 1188 | C    |
| 1   | 1     | 1189 | A    |
| 1   | 1     | 1192 | C    |
| 1   | 1     | 1197 | C    |
| 1   | 1     | 1204 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1205 | G    |
| 1   | 1     | 1218 | G    |
| 1   | 1     | 1223 | C    |
| 1   | 1     | 1224 | C    |
| 1   | 1     | 1229 | G    |
| 1   | 1     | 1230 | G    |
| 1   | 1     | 1231 | U    |
| 1   | 1     | 1232 | G    |
| 1   | 1     | 1239 | G    |
| 1   | 1     | 1240 | A    |
| 1   | 1     | 1241 | A    |
| 1   | 1     | 1242 | G    |
| 1   | 1     | 1243 | U    |
| 1   | 1     | 1244 | C    |
| 1   | 1     | 1245 | G    |
| 1   | 1     | 1246 | G    |
| 1   | 1     | 1247 | A    |
| 1   | 1     | 1249 | U    |
| 1   | 1     | 1250 | C    |
| 1   | 1     | 1252 | G    |
| 1   | 1     | 1254 | U    |
| 1   | 1     | 1255 | A    |
| 1   | 1     | 1257 | G    |
| 1   | 1     | 1258 | G    |
| 1   | 1     | 1259 | A    |
| 1   | 1     | 1262 | G    |
| 1   | 1     | 1263 | U    |
| 1   | 1     | 1264 | G    |
| 1   | 1     | 1265 | U    |
| 1   | 1     | 1266 | A    |
| 1   | 1     | 1269 | A    |
| 1   | 1     | 1270 | A    |
| 1   | 1     | 1271 | C    |
| 1   | 1     | 1273 | C    |
| 1   | 1     | 1274 | A    |
| 1   | 1     | 1278 | G    |
| 1   | 1     | 1303 | G    |
| 1   | 1     | 1304 | A    |
| 1   | 1     | 1305 | U    |
| 1   | 1     | 1309 | G    |
| 1   | 1     | 1312 | C    |
| 1   | 1     | 1326 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1345 | G    |
| 1   | 1     | 1346 | U    |
| 1   | 1     | 1347 | U    |
| 1   | 1     | 1348 | U    |
| 1   | 1     | 1349 | U    |
| 1   | 1     | 1382 | A    |
| 1   | 1     | 1395 | U    |
| 1   | 1     | 1415 | A    |
| 1   | 1     | 1417 | G    |
| 1   | 1     | 1421 | U    |
| 1   | 1     | 1427 | G    |
| 1   | 1     | 1430 | G    |
| 1   | 1     | 1433 | C    |
| 1   | 1     | 1442 | A    |
| 1   | 1     | 1446 | G    |
| 1   | 1     | 1465 | C    |
| 1   | 1     | 1471 | A    |
| 1   | 1     | 1477 | A    |
| 1   | 1     | 1484 | G    |
| 1   | 1     | 1498 | C    |
| 1   | 1     | 1504 | C    |
| 1   | 1     | 1520 | A    |
| 1   | 1     | 1523 | C    |
| 1   | 1     | 1525 | A    |
| 1   | 1     | 1526 | U    |
| 1   | 1     | 1532 | G    |
| 1   | 1     | 1535 | A    |
| 1   | 1     | 1552 | C    |
| 1   | 1     | 1556 | G    |
| 1   | 1     | 1558 | G    |
| 1   | 1     | 1559 | C    |
| 1   | 1     | 1560 | U    |
| 1   | 1     | 1561 | U    |
| 1   | 1     | 1562 | G    |
| 1   | 1     | 1563 | A    |
| 1   | 1     | 1565 | U    |
| 1   | 1     | 1566 | U    |
| 1   | 1     | 1567 | U    |
| 1   | 1     | 1568 | U    |
| 1   | 1     | 1569 | C    |
| 1   | 1     | 1571 | G    |
| 1   | 1     | 1572 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1574 | C    |
| 1   | 1     | 1576 | A    |
| 1   | 1     | 1577 | C    |
| 1   | 1     | 1585 | A    |
| 1   | 1     | 1589 | A    |
| 1   | 1     | 1601 | A    |
| 1   | 1     | 1603 | U    |
| 1   | 1     | 1624 | C    |
| 1   | 1     | 1625 | U    |
| 1   | 1     | 1635 | C    |
| 1   | 1     | 1638 | A    |
| 1   | 1     | 1639 | A    |
| 1   | 1     | 1641 | U    |
| 1   | 1     | 1648 | G    |
| 1   | 1     | 1653 | C    |
| 1   | 1     | 1654 | G    |
| 1   | 1     | 1679 | A    |
| 1   | 1     | 1720 | U    |
| 1   | 1     | 1721 | C    |
| 1   | 1     | 1732 | G    |
| 1   | 1     | 1746 | A    |
| 1   | 1     | 1747 | G    |
| 1   | 1     | 1755 | U    |
| 1   | 1     | 1756 | A    |
| 1   | 1     | 1757 | A    |
| 1   | 1     | 1758 | U    |
| 1   | 1     | 1759 | U    |
| 1   | 1     | 1760 | U    |
| 1   | 1     | 1761 | U    |
| 1   | 1     | 1762 | G    |
| 1   | 1     | 1763 | C    |
| 1   | 1     | 1776 | G    |
| 1   | 1     | 1793 | A    |
| 1   | 1     | 1804 | G    |
| 1   | 1     | 1809 | A    |
| 1   | 1     | 1810 | A    |
| 1   | 1     | 1811 | U    |
| 1   | 1     | 1812 | A    |
| 1   | 1     | 1814 | U    |
| 1   | 1     | 1815 | U    |
| 1   | 1     | 1816 | U    |
| 1   | 1     | 1817 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1837 | A    |
| 1   | 1     | 1838 | A    |
| 1   | 1     | 1842 | C    |
| 1   | 1     | 1845 | C    |
| 1   | 1     | 1862 | C    |
| 1   | 1     | 1874 | G    |
| 1   | 1     | 1882 | A    |
| 1   | 1     | 1889 | A    |
| 1   | 1     | 1902 | G    |
| 1   | 1     | 1944 | G    |
| 1   | 1     | 1949 | G    |
| 1   | 1     | 2068 | U    |
| 1   | 1     | 2069 | U    |
| 1   | 1     | 2070 | A    |
| 1   | 1     | 2071 | A    |
| 1   | 1     | 2078 | A    |
| 1   | 1     | 2088 | G    |
| 1   | 1     | 2089 | G    |
| 1   | 1     | 2091 | A    |
| 1   | 1     | 2092 | C    |
| 1   | 1     | 2099 | G    |
| 1   | 1     | 2100 | G    |
| 1   | 1     | 2109 | A    |
| 1   | 1     | 2118 | U    |
| 1   | 1     | 2122 | A    |
| 1   | 1     | 2136 | A    |
| 1   | 1     | 2147 | G    |
| 1   | 1     | 2149 | G    |
| 1   | 1     | 2183 | U    |
| 1   | 1     | 2184 | G    |
| 1   | 1     | 2185 | A    |
| 1   | 1     | 2186 | A    |
| 1   | 1     | 2187 | U    |
| 1   | 1     | 2188 | G    |
| 1   | 1     | 2222 | A    |
| 1   | 1     | 2227 | G    |
| 1   | 1     | 2233 | A    |
| 1   | 1     | 2234 | A    |
| 1   | 1     | 2235 | C    |
| 1   | 1     | 2250 | G    |
| 1   | 1     | 2251 | G    |
| 1   | 1     | 2259 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2260 | U    |
| 1   | 1     | 2276 | U    |
| 1   | 1     | 2285 | G    |
| 1   | 1     | 2286 | C    |
| 1   | 1     | 2288 | U    |
| 1   | 1     | 2291 | A    |
| 1   | 1     | 2292 | U    |
| 1   | 1     | 2293 | G    |
| 1   | 1     | 2313 | G    |
| 1   | 1     | 2314 | U    |
| 1   | 1     | 2341 | A    |
| 1   | 1     | 2351 | A    |
| 1   | 1     | 2352 | C    |
| 1   | 1     | 2353 | G    |
| 1   | 1     | 2363 | G    |
| 1   | 1     | 2366 | U    |
| 1   | 1     | 2371 | G    |
| 1   | 1     | 2372 | G    |
| 1   | 1     | 2375 | A    |
| 1   | 1     | 2380 | A    |
| 1   | 1     | 2381 | G    |
| 1   | 1     | 2382 | A    |
| 1   | 1     | 2389 | U    |
| 1   | 1     | 2396 | G    |
| 1   | 1     | 2397 | A    |
| 1   | 1     | 2413 | G    |
| 1   | 1     | 2415 | G    |
| 1   | 1     | 2420 | G    |
| 1   | 1     | 2421 | A    |
| 1   | 1     | 2422 | C    |
| 1   | 1     | 2426 | G    |
| 1   | 1     | 2427 | A    |
| 1   | 1     | 2430 | G    |
| 1   | 1     | 2431 | U    |
| 1   | 1     | 2432 | G    |
| 1   | 1     | 2433 | U    |
| 1   | 1     | 2437 | A    |
| 1   | 1     | 2438 | U    |
| 1   | 1     | 2439 | A    |
| 1   | 1     | 2441 | G    |
| 1   | 1     | 2442 | U    |
| 1   | 1     | 2443 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2444 | G    |
| 1   | 1     | 2445 | G    |
| 1   | 1     | 2446 | A    |
| 1   | 1     | 2448 | C    |
| 1   | 1     | 2449 | U    |
| 1   | 1     | 2450 | U    |
| 1   | 1     | 2451 | C    |
| 1   | 1     | 2452 | G    |
| 1   | 1     | 2453 | G    |
| 1   | 1     | 2454 | C    |
| 1   | 1     | 2455 | G    |
| 1   | 1     | 2456 | C    |
| 1   | 1     | 2457 | C    |
| 1   | 1     | 2459 | G    |
| 1   | 1     | 2460 | U    |
| 1   | 1     | 2464 | A    |
| 1   | 1     | 2465 | U    |
| 1   | 1     | 2466 | A    |
| 1   | 1     | 2467 | C    |
| 1   | 1     | 2468 | C    |
| 1   | 1     | 2470 | C    |
| 1   | 1     | 2471 | U    |
| 1   | 1     | 2472 | A    |
| 1   | 1     | 2473 | C    |
| 1   | 1     | 2475 | U    |
| 1   | 1     | 2476 | C    |
| 1   | 1     | 2477 | U    |
| 1   | 1     | 2480 | A    |
| 1   | 1     | 2482 | U    |
| 1   | 1     | 2483 | U    |
| 1   | 1     | 2484 | U    |
| 1   | 1     | 2485 | U    |
| 1   | 1     | 2489 | A    |
| 1   | 1     | 2492 | U    |
| 1   | 1     | 2493 | A    |
| 1   | 1     | 2511 | G    |
| 1   | 1     | 2513 | A    |
| 1   | 1     | 2515 | G    |
| 1   | 1     | 2516 | U    |
| 1   | 1     | 2517 | C    |
| 1   | 1     | 2518 | A    |
| 1   | 1     | 2519 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2520 | A    |
| 1   | 1     | 2521 | C    |
| 1   | 1     | 2529 | U    |
| 1   | 1     | 2530 | C    |
| 1   | 1     | 2533 | G    |
| 1   | 1     | 2536 | U    |
| 1   | 1     | 2538 | A    |
| 1   | 1     | 2545 | C    |
| 1   | 1     | 2546 | U    |
| 1   | 1     | 2554 | C    |
| 1   | 1     | 2557 | G    |
| 1   | 1     | 2565 | A    |
| 1   | 1     | 2566 | C    |
| 1   | 1     | 2578 | G    |
| 1   | 1     | 2579 | G    |
| 1   | 1     | 2586 | G    |
| 1   | 1     | 2598 | A    |
| 1   | 1     | 2623 | G    |
| 1   | 1     | 2624 | U    |
| 1   | 1     | 2628 | A    |
| 1   | 1     | 2644 | G    |
| 1   | 1     | 2646 | A    |
| 1   | 1     | 2649 | G    |
| 1   | 1     | 2661 | A    |
| 1   | 1     | 2662 | G    |
| 1   | 1     | 2663 | A    |
| 1   | 1     | 2664 | A    |
| 1   | 1     | 2666 | A    |
| 1   | 1     | 2668 | A    |
| 1   | 1     | 2676 | A    |
| 1   | 1     | 2677 | A    |
| 1   | 1     | 2686 | G    |
| 1   | 1     | 2691 | U    |
| 1   | 1     | 2699 | A    |
| 1   | 1     | 2700 | G    |
| 1   | 1     | 2701 | U    |
| 1   | 1     | 2724 | U    |
| 1   | 1     | 2725 | G    |
| 1   | 1     | 2734 | A    |
| 1   | 1     | 2745 | C    |
| 1   | 1     | 2749 | G    |
| 1   | 1     | 2750 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2768 | G    |
| 1   | 1     | 2771 | A    |
| 1   | 1     | 2772 | G    |
| 1   | 1     | 2773 | A    |
| 1   | 1     | 2774 | A    |
| 1   | 1     | 2782 | C    |
| 1   | 1     | 2786 | G    |
| 1   | 1     | 2789 | A    |
| 1   | 1     | 2790 | U    |
| 1   | 1     | 2814 | U    |
| 1   | 1     | 2815 | U    |
| 1   | 1     | 2817 | A    |
| 1   | 1     | 2833 | U    |
| 1   | 1     | 2839 | C    |
| 1   | 1     | 2843 | G    |
| 1   | 1     | 2844 | A    |
| 1   | 1     | 2847 | U    |
| 1   | 1     | 2859 | A    |
| 1   | 1     | 2861 | C    |
| 1   | 1     | 2866 | C    |
| 1   | 1     | 2870 | G    |
| 1   | 1     | 2871 | C    |
| 1   | 1     | 2886 | G    |
| 1   | 1     | 2895 | U    |
| 1   | 1     | 2900 | C    |
| 1   | 1     | 2907 | U    |
| 1   | 1     | 2908 | A    |
| 1   | 1     | 2911 | G    |
| 1   | 1     | 2914 | C    |
| 1   | 1     | 2919 | G    |
| 1   | 1     | 2920 | C    |
| 1   | 1     | 2923 | G    |
| 1   | 1     | 2926 | U    |
| 1   | 1     | 2943 | A    |
| 1   | 1     | 2955 | C    |
| 1   | 1     | 2960 | C    |
| 1   | 1     | 2962 | G    |
| 1   | 1     | 2969 | G    |
| 1   | 1     | 2984 | A    |
| 1   | 1     | 3021 | A    |
| 1   | 1     | 3028 | U    |
| 1   | 1     | 3031 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 3050 | A    |
| 1   | 1     | 3051 | C    |
| 1   | 1     | 3052 | G    |
| 1   | 1     | 3058 | A    |
| 1   | 1     | 3064 | C    |
| 1   | 1     | 3073 | G    |
| 1   | 1     | 3094 | A    |
| 1   | 1     | 3101 | A    |
| 1   | 1     | 3102 | A    |
| 1   | 1     | 3103 | U    |
| 1   | 1     | 3114 | A    |
| 1   | 1     | 3115 | C    |
| 1   | 1     | 3125 | U    |
| 1   | 1     | 3127 | U    |
| 1   | 1     | 3143 | G    |
| 1   | 1     | 3144 | A    |
| 1   | 1     | 3146 | G    |
| 1   | 1     | 3149 | U    |
| 1   | 1     | 3151 | C    |
| 1   | 1     | 3157 | A    |
| 1   | 1     | 3160 | C    |
| 1   | 1     | 3161 | U    |
| 1   | 1     | 3162 | U    |
| 1   | 1     | 3163 | U    |
| 1   | 1     | 3164 | U    |
| 1   | 1     | 3165 | U    |
| 1   | 1     | 3166 | A    |
| 1   | 1     | 3171 | C    |
| 1   | 1     | 3172 | U    |
| 1   | 1     | 3182 | C    |
| 1   | 1     | 3183 | A    |
| 1   | 1     | 3184 | G    |
| 1   | 1     | 3194 | G    |
| 1   | 1     | 3208 | A    |
| 1   | 1     | 3210 | A    |
| 1   | 1     | 3212 | G    |
| 1   | 1     | 3214 | U    |
| 1   | 1     | 3221 | G    |
| 1   | 1     | 3224 | U    |
| 1   | 1     | 3228 | G    |
| 1   | 1     | 3235 | A    |
| 1   | 1     | 3241 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 3246 | C    |
| 1   | 1     | 3252 | C    |
| 1   | 1     | 3259 | A    |
| 1   | 1     | 3260 | A    |
| 1   | 1     | 3268 | G    |
| 1   | 1     | 3269 | C    |
| 1   | 1     | 3272 | A    |
| 1   | 1     | 3278 | U    |
| 1   | 1     | 3281 | A    |
| 1   | 1     | 3284 | U    |
| 1   | 1     | 3285 | A    |
| 1   | 1     | 3306 | U    |
| 1   | 1     | 3307 | A    |
| 1   | 1     | 3309 | A    |
| 1   | 1     | 3310 | G    |
| 1   | 1     | 3316 | U    |
| 1   | 1     | 3317 | U    |
| 1   | 1     | 3318 | G    |
| 1   | 1     | 3319 | U    |
| 1   | 1     | 3320 | U    |
| 1   | 1     | 3321 | G    |
| 1   | 1     | 3334 | G    |
| 1   | 1     | 3343 | C    |
| 1   | 1     | 3351 | G    |
| 1   | 1     | 3361 | U    |
| 2   | 3     | 7    | G    |
| 2   | 3     | 22   | A    |
| 2   | 3     | 54   | U    |
| 2   | 3     | 55   | A    |
| 2   | 3     | 65   | G    |
| 2   | 3     | 73   | C    |
| 2   | 3     | 76   | A    |
| 2   | 3     | 102  | A    |
| 2   | 3     | 112  | G    |
| 3   | 4     | 23   | U    |
| 3   | 4     | 34   | U    |
| 3   | 4     | 35   | C    |
| 3   | 4     | 59   | A    |
| 3   | 4     | 62   | C    |
| 3   | 4     | 63   | G    |
| 3   | 4     | 81   | A    |
| 3   | 4     | 84   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 4     | 85  | G    |
| 3   | 4     | 86  | U    |
| 3   | 4     | 87  | G    |
| 3   | 4     | 92  | A    |
| 3   | 4     | 95  | G    |
| 3   | 4     | 102 | U    |
| 3   | 4     | 104 | A    |
| 3   | 4     | 106 | C    |
| 3   | 4     | 111 | A    |
| 3   | 4     | 113 | U    |
| 3   | 4     | 125 | U    |
| 3   | 4     | 126 | A    |
| 3   | 4     | 148 | G    |
| 3   | 4     | 152 | G    |
| 46  | B     | 17  | C    |
| 46  | B     | 25  | C    |
| 46  | B     | 26  | A    |
| 46  | B     | 27  | U    |
| 46  | B     | 34  | G    |
| 46  | B     | 47  | A    |
| 46  | B     | 57  | G    |
| 46  | B     | 66  | U    |
| 46  | B     | 74  | U    |
| 46  | B     | 75  | U    |
| 46  | B     | 76  | A    |
| 46  | B     | 78  | A    |
| 46  | B     | 79  | C    |
| 46  | B     | 81  | G    |
| 46  | B     | 84  | A    |
| 46  | B     | 93  | A    |
| 46  | B     | 104 | A    |
| 46  | B     | 114 | C    |
| 46  | B     | 115 | G    |
| 46  | B     | 123 | G    |
| 46  | B     | 126 | A    |
| 46  | B     | 127 | G    |
| 46  | B     | 128 | U    |
| 46  | B     | 138 | C    |
| 46  | B     | 139 | U    |
| 46  | B     | 142 | G    |
| 46  | B     | 143 | A    |
| 46  | B     | 150 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | B     | 151 | G    |
| 46  | B     | 152 | G    |
| 46  | B     | 154 | A    |
| 46  | B     | 159 | U    |
| 46  | B     | 166 | A    |
| 46  | B     | 168 | U    |
| 46  | B     | 173 | G    |
| 46  | B     | 174 | C    |
| 46  | B     | 176 | U    |
| 46  | B     | 177 | A    |
| 46  | B     | 179 | A    |
| 46  | B     | 190 | U    |
| 46  | B     | 191 | U    |
| 46  | B     | 193 | G    |
| 46  | B     | 199 | G    |
| 46  | B     | 200 | A    |
| 46  | B     | 202 | G    |
| 46  | B     | 206 | U    |
| 46  | B     | 211 | A    |
| 46  | B     | 213 | A    |
| 46  | B     | 214 | U    |
| 46  | B     | 215 | A    |
| 46  | B     | 216 | A    |
| 46  | B     | 217 | A    |
| 46  | B     | 218 | A    |
| 46  | B     | 224 | A    |
| 46  | B     | 226 | G    |
| 46  | B     | 229 | U    |
| 46  | B     | 230 | U    |
| 46  | B     | 231 | C    |
| 46  | B     | 236 | U    |
| 46  | B     | 237 | C    |
| 46  | B     | 247 | U    |
| 46  | B     | 255 | A    |
| 46  | B     | 259 | U    |
| 46  | B     | 260 | U    |
| 46  | B     | 261 | C    |
| 46  | B     | 262 | G    |
| 46  | B     | 266 | C    |
| 46  | B     | 269 | A    |
| 46  | B     | 270 | U    |
| 46  | B     | 274 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | B     | 276 | U    |
| 46  | B     | 277 | G    |
| 46  | B     | 278 | U    |
| 46  | B     | 279 | G    |
| 46  | B     | 283 | G    |
| 46  | B     | 285 | G    |
| 46  | B     | 297 | A    |
| 46  | B     | 312 | C    |
| 46  | B     | 314 | A    |
| 46  | B     | 318 | U    |
| 46  | B     | 319 | C    |
| 46  | B     | 320 | G    |
| 46  | B     | 335 | G    |
| 46  | B     | 336 | C    |
| 46  | B     | 350 | A    |
| 46  | B     | 357 | A    |
| 46  | B     | 358 | A    |
| 46  | B     | 359 | C    |
| 46  | B     | 388 | G    |
| 46  | B     | 398 | A    |
| 46  | B     | 400 | C    |
| 46  | B     | 402 | G    |
| 46  | B     | 414 | A    |
| 46  | B     | 416 | G    |
| 46  | B     | 421 | G    |
| 46  | B     | 422 | C    |
| 46  | B     | 423 | A    |
| 46  | B     | 424 | G    |
| 46  | B     | 432 | G    |
| 46  | B     | 437 | U    |
| 46  | B     | 442 | C    |
| 46  | B     | 446 | C    |
| 46  | B     | 452 | A    |
| 46  | B     | 458 | A    |
| 46  | B     | 466 | A    |
| 46  | B     | 475 | A    |
| 46  | B     | 480 | U    |
| 46  | B     | 483 | A    |
| 46  | B     | 485 | G    |
| 46  | B     | 487 | C    |
| 46  | B     | 490 | U    |
| 46  | B     | 491 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | B     | 493 | U    |
| 46  | B     | 499 | U    |
| 46  | B     | 503 | A    |
| 46  | B     | 505 | U    |
| 46  | B     | 506 | U    |
| 46  | B     | 509 | A    |
| 46  | B     | 512 | G    |
| 46  | B     | 513 | A    |
| 46  | B     | 515 | U    |
| 46  | B     | 518 | A    |
| 46  | B     | 519 | A    |
| 46  | B     | 525 | A    |
| 46  | B     | 530 | U    |
| 46  | B     | 534 | C    |
| 46  | B     | 536 | A    |
| 46  | B     | 537 | G    |
| 46  | B     | 539 | A    |
| 46  | B     | 540 | A    |
| 46  | B     | 547 | G    |
| 46  | B     | 553 | A    |
| 46  | B     | 554 | A    |
| 46  | B     | 555 | G    |
| 46  | B     | 556 | U    |
| 46  | B     | 557 | C    |
| 46  | B     | 563 | C    |
| 46  | B     | 566 | G    |
| 46  | B     | 575 | G    |
| 46  | B     | 576 | U    |
| 46  | B     | 580 | U    |
| 46  | B     | 592 | A    |
| 46  | B     | 593 | G    |
| 46  | B     | 604 | A    |
| 46  | B     | 609 | U    |
| 46  | B     | 617 | A    |
| 46  | B     | 618 | A    |
| 46  | B     | 620 | A    |
| 46  | B     | 621 | A    |
| 46  | B     | 639 | G    |
| 46  | B     | 643 | U    |
| 46  | B     | 645 | G    |
| 46  | B     | 647 | C    |
| 46  | B     | 648 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | B     | 649 | G    |
| 46  | B     | 650 | G    |
| 46  | B     | 651 | C    |
| 46  | B     | 652 | C    |
| 46  | B     | 653 | G    |
| 46  | B     | 657 | C    |
| 46  | B     | 670 | C    |
| 46  | B     | 671 | G    |
| 46  | B     | 672 | U    |
| 46  | B     | 673 | A    |
| 46  | B     | 674 | C    |
| 46  | B     | 675 | U    |
| 46  | B     | 677 | G    |
| 46  | B     | 678 | A    |
| 46  | B     | 679 | C    |
| 46  | B     | 680 | C    |
| 46  | B     | 681 | C    |
| 46  | B     | 682 | A    |
| 46  | B     | 688 | G    |
| 46  | B     | 695 | C    |
| 46  | B     | 729 | U    |
| 46  | B     | 739 | A    |
| 46  | B     | 740 | A    |
| 46  | B     | 741 | A    |
| 46  | B     | 750 | G    |
| 46  | B     | 751 | U    |
| 46  | B     | 756 | A    |
| 46  | B     | 759 | A    |
| 46  | B     | 760 | G    |
| 46  | B     | 762 | C    |
| 46  | B     | 764 | U    |
| 46  | B     | 765 | U    |
| 46  | B     | 766 | U    |
| 46  | B     | 767 | G    |
| 46  | B     | 768 | C    |
| 46  | B     | 770 | C    |
| 46  | B     | 771 | G    |
| 46  | B     | 773 | A    |
| 46  | B     | 775 | A    |
| 46  | B     | 778 | U    |
| 46  | B     | 779 | U    |
| 46  | B     | 796 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | B     | 798 | A    |
| 46  | B     | 799 | G    |
| 46  | B     | 802 | C    |
| 46  | B     | 803 | G    |
| 46  | B     | 804 | U    |
| 46  | B     | 805 | U    |
| 46  | B     | 807 | U    |
| 46  | B     | 808 | G    |
| 46  | B     | 813 | U    |
| 46  | B     | 815 | U    |
| 46  | B     | 817 | U    |
| 46  | B     | 819 | G    |
| 46  | B     | 820 | U    |
| 46  | B     | 821 | U    |
| 46  | B     | 823 | G    |
| 46  | B     | 824 | U    |
| 46  | B     | 825 | U    |
| 46  | B     | 826 | U    |
| 46  | B     | 827 | C    |
| 46  | B     | 828 | U    |
| 46  | B     | 829 | A    |
| 46  | B     | 831 | G    |
| 46  | B     | 840 | A    |
| 46  | B     | 842 | U    |
| 46  | B     | 847 | A    |
| 46  | B     | 848 | A    |
| 46  | B     | 856 | G    |
| 46  | B     | 857 | G    |
| 46  | B     | 869 | A    |
| 46  | B     | 871 | U    |
| 46  | B     | 875 | C    |
| 46  | B     | 877 | G    |
| 46  | B     | 878 | U    |
| 46  | B     | 879 | U    |
| 46  | B     | 881 | U    |
| 46  | B     | 891 | A    |
| 46  | B     | 909 | A    |
| 46  | B     | 910 | G    |
| 46  | B     | 911 | A    |
| 46  | B     | 918 | A    |
| 46  | B     | 920 | U    |
| 46  | B     | 927 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | B     | 945  | U    |
| 46  | B     | 951  | A    |
| 46  | B     | 973  | A    |
| 46  | B     | 975  | C    |
| 46  | B     | 977  | A    |
| 46  | B     | 988  | A    |
| 46  | B     | 989  | U    |
| 46  | B     | 990  | A    |
| 46  | B     | 997  | U    |
| 46  | B     | 998  | A    |
| 46  | B     | 1004 | A    |
| 46  | B     | 1005 | A    |
| 46  | B     | 1011 | A    |
| 46  | B     | 1013 | C    |
| 46  | B     | 1017 | G    |
| 46  | B     | 1024 | A    |
| 46  | B     | 1025 | G    |
| 46  | B     | 1039 | U    |
| 46  | B     | 1042 | U    |
| 46  | B     | 1043 | U    |
| 46  | B     | 1055 | A    |
| 46  | B     | 1056 | U    |
| 46  | B     | 1057 | C    |
| 46  | B     | 1058 | G    |
| 46  | B     | 1059 | G    |
| 46  | B     | 1060 | C    |
| 46  | B     | 1061 | A    |
| 46  | B     | 1067 | C    |
| 46  | B     | 1077 | A    |
| 46  | B     | 1081 | C    |
| 46  | B     | 1085 | G    |
| 46  | B     | 1123 | A    |
| 46  | B     | 1135 | G    |
| 46  | B     | 1143 | C    |
| 46  | B     | 1145 | A    |
| 46  | B     | 1152 | G    |
| 46  | B     | 1168 | A    |
| 46  | B     | 1169 | A    |
| 46  | B     | 1170 | U    |
| 46  | B     | 1179 | A    |
| 46  | B     | 1181 | A    |
| 46  | B     | 1184 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | B     | 1185 | G    |
| 46  | B     | 1186 | G    |
| 46  | B     | 1187 | A    |
| 46  | B     | 1193 | A    |
| 46  | B     | 1202 | A    |
| 46  | B     | 1203 | G    |
| 46  | B     | 1206 | A    |
| 46  | B     | 1207 | C    |
| 46  | B     | 1212 | A    |
| 46  | B     | 1215 | A    |
| 46  | B     | 1219 | A    |
| 46  | B     | 1220 | C    |
| 46  | B     | 1221 | A    |
| 46  | B     | 1229 | A    |
| 46  | B     | 1230 | G    |
| 46  | B     | 1231 | C    |
| 46  | B     | 1236 | U    |
| 46  | B     | 1243 | U    |
| 46  | B     | 1250 | G    |
| 46  | B     | 1270 | U    |
| 46  | B     | 1299 | U    |
| 46  | B     | 1300 | U    |
| 46  | B     | 1301 | G    |
| 46  | B     | 1306 | A    |
| 46  | B     | 1325 | U    |
| 46  | B     | 1330 | A    |
| 46  | B     | 1336 | G    |
| 46  | B     | 1339 | G    |
| 46  | B     | 1342 | A    |
| 46  | B     | 1343 | G    |
| 46  | B     | 1345 | A    |
| 46  | B     | 1346 | U    |
| 46  | B     | 1348 | U    |
| 46  | B     | 1349 | G    |
| 46  | B     | 1352 | G    |
| 46  | B     | 1355 | A    |
| 46  | B     | 1356 | U    |
| 46  | B     | 1357 | A    |
| 46  | B     | 1359 | U    |
| 46  | B     | 1360 | C    |
| 46  | B     | 1364 | U    |
| 46  | B     | 1369 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | B     | 1370 | A    |
| 46  | B     | 1376 | U    |
| 46  | B     | 1380 | G    |
| 46  | B     | 1381 | A    |
| 46  | B     | 1382 | U    |
| 46  | B     | 1384 | U    |
| 46  | B     | 1385 | C    |
| 46  | B     | 1392 | A    |
| 46  | B     | 1397 | A    |
| 46  | B     | 1398 | G    |
| 46  | B     | 1399 | U    |
| 46  | B     | 1400 | U    |
| 46  | B     | 1401 | U    |
| 46  | B     | 1410 | A    |
| 46  | B     | 1413 | A    |
| 46  | B     | 1414 | G    |
| 46  | B     | 1415 | G    |
| 46  | B     | 1422 | A    |
| 46  | B     | 1431 | G    |
| 46  | B     | 1433 | C    |
| 46  | B     | 1445 | C    |
| 46  | B     | 1446 | A    |
| 46  | B     | 1455 | A    |
| 46  | B     | 1457 | A    |
| 46  | B     | 1458 | C    |
| 46  | B     | 1461 | A    |
| 46  | B     | 1462 | C    |
| 46  | B     | 1463 | G    |
| 46  | B     | 1468 | C    |
| 46  | B     | 1476 | A    |
| 46  | B     | 1477 | U    |
| 46  | B     | 1480 | G    |
| 46  | B     | 1483 | U    |
| 46  | B     | 1485 | G    |
| 46  | B     | 1491 | G    |
| 46  | B     | 1502 | A    |
| 46  | B     | 1503 | A    |
| 46  | B     | 1508 | G    |
| 46  | B     | 1510 | G    |
| 46  | B     | 1511 | A    |
| 46  | B     | 1523 | G    |
| 46  | B     | 1524 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | B     | 1529 | G    |
| 46  | B     | 1530 | A    |
| 46  | B     | 1541 | U    |
| 46  | B     | 1544 | U    |
| 46  | B     | 1546 | G    |
| 46  | B     | 1560 | A    |
| 46  | B     | 1561 | G    |
| 46  | B     | 1571 | G    |
| 46  | B     | 1574 | A    |
| 46  | B     | 1575 | G    |
| 46  | B     | 1577 | G    |
| 46  | B     | 1580 | A    |
| 46  | B     | 1582 | U    |
| 46  | B     | 1584 | A    |
| 46  | B     | 1588 | G    |
| 46  | B     | 1621 | C    |
| 46  | B     | 1644 | U    |
| 46  | B     | 1645 | G    |
| 46  | B     | 1665 | C    |
| 46  | B     | 1667 | G    |
| 46  | B     | 1670 | U    |
| 46  | B     | 1671 | G    |
| 46  | B     | 1672 | G    |
| 46  | B     | 1673 | U    |
| 46  | B     | 1702 | A    |
| 46  | B     | 1704 | C    |
| 46  | B     | 1737 | A    |
| 46  | B     | 1742 | A    |
| 46  | B     | 1743 | A    |
| 46  | B     | 1744 | G    |
| 46  | B     | 1747 | G    |
| 46  | B     | 1749 | A    |
| 46  | B     | 1753 | A    |
| 46  | B     | 1756 | U    |
| 46  | B     | 1767 | G    |
| 46  | B     | 1770 | C    |
| 46  | B     | 1779 | G    |
| 46  | B     | 1780 | G    |
| 46  | B     | 1781 | A    |
| 46  | B     | 1782 | U    |
| 46  | B     | 1783 | C    |
| 1   | AS    | 24   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AS    | 25  | A    |
| 1   | AS    | 29  | G    |
| 1   | AS    | 39  | A    |
| 1   | AS    | 42  | A    |
| 1   | AS    | 48  | A    |
| 1   | AS    | 56  | A    |
| 1   | AS    | 58  | G    |
| 1   | AS    | 59  | A    |
| 1   | AS    | 64  | A    |
| 1   | AS    | 65  | A    |
| 1   | AS    | 91  | G    |
| 1   | AS    | 98  | A    |
| 1   | AS    | 104 | C    |
| 1   | AS    | 108 | A    |
| 1   | AS    | 109 | G    |
| 1   | AS    | 110 | C    |
| 1   | AS    | 121 | A    |
| 1   | AS    | 134 | U    |
| 1   | AS    | 135 | G    |
| 1   | AS    | 155 | A    |
| 1   | AS    | 156 | A    |
| 1   | AS    | 164 | U    |
| 1   | AS    | 169 | G    |
| 1   | AS    | 172 | C    |
| 1   | AS    | 173 | C    |
| 1   | AS    | 175 | G    |
| 1   | AS    | 186 | A    |
| 1   | AS    | 189 | U    |
| 1   | AS    | 190 | U    |
| 1   | AS    | 199 | C    |
| 1   | AS    | 205 | G    |
| 1   | AS    | 209 | C    |
| 1   | AS    | 212 | A    |
| 1   | AS    | 217 | G    |
| 1   | AS    | 218 | A    |
| 1   | AS    | 219 | G    |
| 1   | AS    | 230 | G    |
| 1   | AS    | 236 | A    |
| 1   | AS    | 239 | A    |
| 1   | AS    | 240 | C    |
| 1   | AS    | 243 | G    |
| 1   | AS    | 245 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AS    | 249 | G    |
| 1   | AS    | 250 | U    |
| 1   | AS    | 269 | G    |
| 1   | AS    | 286 | U    |
| 1   | AS    | 295 | A    |
| 1   | AS    | 305 | U    |
| 1   | AS    | 311 | C    |
| 1   | AS    | 323 | A    |
| 1   | AS    | 329 | U    |
| 1   | AS    | 337 | G    |
| 1   | AS    | 338 | A    |
| 1   | AS    | 339 | C    |
| 1   | AS    | 343 | U    |
| 1   | AS    | 349 | A    |
| 1   | AS    | 350 | C    |
| 1   | AS    | 376 | G    |
| 1   | AS    | 377 | A    |
| 1   | AS    | 395 | A    |
| 1   | AS    | 398 | A    |
| 1   | AS    | 402 | A    |
| 1   | AS    | 403 | C    |
| 1   | AS    | 404 | G    |
| 1   | AS    | 420 | G    |
| 1   | AS    | 421 | G    |
| 1   | AS    | 422 | A    |
| 1   | AS    | 438 | A    |
| 1   | AS    | 439 | C    |
| 1   | AS    | 445 | A    |
| 1   | AS    | 447 | U    |
| 1   | AS    | 448 | U    |
| 1   | AS    | 449 | U    |
| 1   | AS    | 450 | G    |
| 1   | AS    | 451 | C    |
| 1   | AS    | 478 | G    |
| 1   | AS    | 479 | C    |
| 1   | AS    | 480 | G    |
| 1   | AS    | 481 | G    |
| 1   | AS    | 482 | U    |
| 1   | AS    | 483 | U    |
| 1   | AS    | 484 | U    |
| 1   | AS    | 486 | C    |
| 1   | AS    | 487 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AS    | 488 | G    |
| 1   | AS    | 506 | A    |
| 1   | AS    | 517 | A    |
| 1   | AS    | 519 | U    |
| 1   | AS    | 531 | G    |
| 1   | AS    | 532 | U    |
| 1   | AS    | 538 | G    |
| 1   | AS    | 539 | G    |
| 1   | AS    | 540 | C    |
| 1   | AS    | 541 | U    |
| 1   | AS    | 555 | A    |
| 1   | AS    | 556 | U    |
| 1   | AS    | 557 | A    |
| 1   | AS    | 564 | G    |
| 1   | AS    | 576 | A    |
| 1   | AS    | 577 | G    |
| 1   | AS    | 589 | G    |
| 1   | AS    | 590 | A    |
| 1   | AS    | 598 | U    |
| 1   | AS    | 600 | U    |
| 1   | AS    | 601 | U    |
| 1   | AS    | 602 | A    |
| 1   | AS    | 609 | A    |
| 1   | AS    | 618 | U    |
| 1   | AS    | 619 | A    |
| 1   | AS    | 620 | A    |
| 1   | AS    | 635 | C    |
| 1   | AS    | 647 | A    |
| 1   | AS    | 658 | A    |
| 1   | AS    | 675 | A    |
| 1   | AS    | 679 | U    |
| 1   | AS    | 688 | A    |
| 1   | AS    | 689 | A    |
| 1   | AS    | 703 | A    |
| 1   | AS    | 710 | G    |
| 1   | AS    | 713 | A    |
| 1   | AS    | 717 | A    |
| 1   | AS    | 723 | G    |
| 1   | AS    | 730 | A    |
| 1   | AS    | 732 | U    |
| 1   | AS    | 760 | U    |
| 1   | AS    | 763 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 772  | U    |
| 1   | AS    | 773  | U    |
| 1   | AS    | 776  | A    |
| 1   | AS    | 777  | G    |
| 1   | AS    | 780  | A    |
| 1   | AS    | 781  | G    |
| 1   | AS    | 802  | A    |
| 1   | AS    | 813  | A    |
| 1   | AS    | 826  | A    |
| 1   | AS    | 845  | C    |
| 1   | AS    | 857  | C    |
| 1   | AS    | 861  | U    |
| 1   | AS    | 870  | U    |
| 1   | AS    | 875  | U    |
| 1   | AS    | 892  | A    |
| 1   | AS    | 903  | G    |
| 1   | AS    | 904  | G    |
| 1   | AS    | 910  | A    |
| 1   | AS    | 912  | G    |
| 1   | AS    | 913  | A    |
| 1   | AS    | 917  | A    |
| 1   | AS    | 919  | C    |
| 1   | AS    | 921  | A    |
| 1   | AS    | 933  | G    |
| 1   | AS    | 940  | C    |
| 1   | AS    | 949  | G    |
| 1   | AS    | 955  | C    |
| 1   | AS    | 956  | U    |
| 1   | AS    | 959  | G    |
| 1   | AS    | 970  | G    |
| 1   | AS    | 976  | A    |
| 1   | AS    | 977  | U    |
| 1   | AS    | 990  | G    |
| 1   | AS    | 991  | U    |
| 1   | AS    | 996  | C    |
| 1   | AS    | 997  | G    |
| 1   | AS    | 998  | A    |
| 1   | AS    | 1006 | G    |
| 1   | AS    | 1011 | C    |
| 1   | AS    | 1012 | U    |
| 1   | AS    | 1014 | G    |
| 1   | AS    | 1019 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 1020 | G    |
| 1   | AS    | 1026 | A    |
| 1   | AS    | 1027 | C    |
| 1   | AS    | 1030 | U    |
| 1   | AS    | 1033 | C    |
| 1   | AS    | 1043 | A    |
| 1   | AS    | 1045 | C    |
| 1   | AS    | 1060 | A    |
| 1   | AS    | 1061 | A    |
| 1   | AS    | 1068 | G    |
| 1   | AS    | 1077 | U    |
| 1   | AS    | 1078 | U    |
| 1   | AS    | 1089 | A    |
| 1   | AS    | 1090 | A    |
| 1   | AS    | 1091 | U    |
| 1   | AS    | 1092 | U    |
| 1   | AS    | 1094 | A    |
| 1   | AS    | 1099 | A    |
| 1   | AS    | 1100 | G    |
| 1   | AS    | 1113 | G    |
| 1   | AS    | 1127 | G    |
| 1   | AS    | 1140 | U    |
| 1   | AS    | 1149 | A    |
| 1   | AS    | 1150 | A    |
| 1   | AS    | 1151 | C    |
| 1   | AS    | 1155 | A    |
| 1   | AS    | 1156 | C    |
| 1   | AS    | 1164 | U    |
| 1   | AS    | 1174 | G    |
| 1   | AS    | 1176 | A    |
| 1   | AS    | 1177 | U    |
| 1   | AS    | 1178 | G    |
| 1   | AS    | 1188 | C    |
| 1   | AS    | 1189 | A    |
| 1   | AS    | 1192 | C    |
| 1   | AS    | 1197 | C    |
| 1   | AS    | 1204 | U    |
| 1   | AS    | 1205 | G    |
| 1   | AS    | 1218 | G    |
| 1   | AS    | 1219 | A    |
| 1   | AS    | 1224 | C    |
| 1   | AS    | 1228 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 1303 | G    |
| 1   | AS    | 1304 | A    |
| 1   | AS    | 1305 | U    |
| 1   | AS    | 1309 | G    |
| 1   | AS    | 1326 | A    |
| 1   | AS    | 1345 | G    |
| 1   | AS    | 1346 | U    |
| 1   | AS    | 1347 | U    |
| 1   | AS    | 1348 | U    |
| 1   | AS    | 1382 | A    |
| 1   | AS    | 1395 | U    |
| 1   | AS    | 1415 | A    |
| 1   | AS    | 1417 | G    |
| 1   | AS    | 1421 | U    |
| 1   | AS    | 1427 | G    |
| 1   | AS    | 1430 | G    |
| 1   | AS    | 1433 | C    |
| 1   | AS    | 1442 | A    |
| 1   | AS    | 1446 | G    |
| 1   | AS    | 1465 | C    |
| 1   | AS    | 1471 | A    |
| 1   | AS    | 1477 | A    |
| 1   | AS    | 1484 | G    |
| 1   | AS    | 1498 | C    |
| 1   | AS    | 1504 | C    |
| 1   | AS    | 1520 | A    |
| 1   | AS    | 1523 | C    |
| 1   | AS    | 1532 | G    |
| 1   | AS    | 1535 | A    |
| 1   | AS    | 1552 | C    |
| 1   | AS    | 1556 | G    |
| 1   | AS    | 1558 | G    |
| 1   | AS    | 1559 | C    |
| 1   | AS    | 1560 | U    |
| 1   | AS    | 1561 | U    |
| 1   | AS    | 1562 | G    |
| 1   | AS    | 1563 | A    |
| 1   | AS    | 1564 | U    |
| 1   | AS    | 1568 | U    |
| 1   | AS    | 1569 | C    |
| 1   | AS    | 1571 | G    |
| 1   | AS    | 1572 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 1574 | C    |
| 1   | AS    | 1576 | A    |
| 1   | AS    | 1577 | C    |
| 1   | AS    | 1585 | A    |
| 1   | AS    | 1589 | A    |
| 1   | AS    | 1601 | A    |
| 1   | AS    | 1603 | U    |
| 1   | AS    | 1624 | C    |
| 1   | AS    | 1625 | U    |
| 1   | AS    | 1635 | C    |
| 1   | AS    | 1638 | A    |
| 1   | AS    | 1639 | A    |
| 1   | AS    | 1641 | U    |
| 1   | AS    | 1648 | G    |
| 1   | AS    | 1654 | G    |
| 1   | AS    | 1679 | A    |
| 1   | AS    | 1720 | U    |
| 1   | AS    | 1721 | C    |
| 1   | AS    | 1732 | G    |
| 1   | AS    | 1746 | A    |
| 1   | AS    | 1747 | G    |
| 1   | AS    | 1755 | U    |
| 1   | AS    | 1756 | A    |
| 1   | AS    | 1757 | A    |
| 1   | AS    | 1758 | U    |
| 1   | AS    | 1759 | U    |
| 1   | AS    | 1761 | U    |
| 1   | AS    | 1762 | G    |
| 1   | AS    | 1763 | C    |
| 1   | AS    | 1776 | G    |
| 1   | AS    | 1793 | A    |
| 1   | AS    | 1804 | G    |
| 1   | AS    | 1809 | A    |
| 1   | AS    | 1810 | A    |
| 1   | AS    | 1811 | U    |
| 1   | AS    | 1812 | A    |
| 1   | AS    | 1814 | U    |
| 1   | AS    | 1815 | U    |
| 1   | AS    | 1816 | U    |
| 1   | AS    | 1817 | U    |
| 1   | AS    | 1835 | A    |
| 1   | AS    | 1838 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 1842 | C    |
| 1   | AS    | 1845 | C    |
| 1   | AS    | 1862 | C    |
| 1   | AS    | 1874 | G    |
| 1   | AS    | 1882 | A    |
| 1   | AS    | 1889 | A    |
| 1   | AS    | 1902 | G    |
| 1   | AS    | 1944 | G    |
| 1   | AS    | 1949 | G    |
| 1   | AS    | 2071 | A    |
| 1   | AS    | 2078 | A    |
| 1   | AS    | 2088 | G    |
| 1   | AS    | 2089 | G    |
| 1   | AS    | 2091 | A    |
| 1   | AS    | 2092 | C    |
| 1   | AS    | 2099 | G    |
| 1   | AS    | 2100 | G    |
| 1   | AS    | 2109 | A    |
| 1   | AS    | 2118 | U    |
| 1   | AS    | 2122 | A    |
| 1   | AS    | 2136 | A    |
| 1   | AS    | 2147 | G    |
| 1   | AS    | 2149 | G    |
| 1   | AS    | 2183 | U    |
| 1   | AS    | 2184 | G    |
| 1   | AS    | 2185 | A    |
| 1   | AS    | 2186 | A    |
| 1   | AS    | 2187 | U    |
| 1   | AS    | 2188 | G    |
| 1   | AS    | 2201 | A    |
| 1   | AS    | 2222 | A    |
| 1   | AS    | 2227 | G    |
| 1   | AS    | 2233 | A    |
| 1   | AS    | 2234 | A    |
| 1   | AS    | 2250 | G    |
| 1   | AS    | 2251 | G    |
| 1   | AS    | 2257 | A    |
| 1   | AS    | 2259 | A    |
| 1   | AS    | 2260 | U    |
| 1   | AS    | 2276 | U    |
| 1   | AS    | 2285 | G    |
| 1   | AS    | 2286 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 2288 | U    |
| 1   | AS    | 2291 | A    |
| 1   | AS    | 2292 | U    |
| 1   | AS    | 2293 | G    |
| 1   | AS    | 2312 | U    |
| 1   | AS    | 2313 | G    |
| 1   | AS    | 2314 | U    |
| 1   | AS    | 2341 | A    |
| 1   | AS    | 2351 | A    |
| 1   | AS    | 2352 | C    |
| 1   | AS    | 2353 | G    |
| 1   | AS    | 2363 | G    |
| 1   | AS    | 2366 | U    |
| 1   | AS    | 2371 | G    |
| 1   | AS    | 2372 | G    |
| 1   | AS    | 2375 | A    |
| 1   | AS    | 2380 | A    |
| 1   | AS    | 2381 | G    |
| 1   | AS    | 2382 | A    |
| 1   | AS    | 2389 | U    |
| 1   | AS    | 2396 | G    |
| 1   | AS    | 2397 | A    |
| 1   | AS    | 2413 | G    |
| 1   | AS    | 2419 | A    |
| 1   | AS    | 2421 | A    |
| 1   | AS    | 2422 | C    |
| 1   | AS    | 2425 | G    |
| 1   | AS    | 2426 | G    |
| 1   | AS    | 2427 | A    |
| 1   | AS    | 2428 | G    |
| 1   | AS    | 2429 | G    |
| 1   | AS    | 2430 | G    |
| 1   | AS    | 2431 | U    |
| 1   | AS    | 2482 | U    |
| 1   | AS    | 2483 | U    |
| 1   | AS    | 2484 | U    |
| 1   | AS    | 2489 | A    |
| 1   | AS    | 2492 | U    |
| 1   | AS    | 2493 | A    |
| 1   | AS    | 2510 | U    |
| 1   | AS    | 2511 | G    |
| 1   | AS    | 2513 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 2515 | G    |
| 1   | AS    | 2516 | U    |
| 1   | AS    | 2517 | C    |
| 1   | AS    | 2518 | A    |
| 1   | AS    | 2519 | A    |
| 1   | AS    | 2520 | A    |
| 1   | AS    | 2521 | C    |
| 1   | AS    | 2529 | U    |
| 1   | AS    | 2530 | C    |
| 1   | AS    | 2533 | G    |
| 1   | AS    | 2536 | U    |
| 1   | AS    | 2538 | A    |
| 1   | AS    | 2545 | C    |
| 1   | AS    | 2546 | U    |
| 1   | AS    | 2554 | C    |
| 1   | AS    | 2557 | G    |
| 1   | AS    | 2565 | A    |
| 1   | AS    | 2566 | C    |
| 1   | AS    | 2578 | G    |
| 1   | AS    | 2579 | G    |
| 1   | AS    | 2586 | G    |
| 1   | AS    | 2598 | A    |
| 1   | AS    | 2623 | G    |
| 1   | AS    | 2624 | U    |
| 1   | AS    | 2628 | A    |
| 1   | AS    | 2646 | A    |
| 1   | AS    | 2649 | G    |
| 1   | AS    | 2661 | A    |
| 1   | AS    | 2662 | G    |
| 1   | AS    | 2663 | A    |
| 1   | AS    | 2666 | A    |
| 1   | AS    | 2668 | A    |
| 1   | AS    | 2676 | A    |
| 1   | AS    | 2677 | A    |
| 1   | AS    | 2686 | G    |
| 1   | AS    | 2699 | A    |
| 1   | AS    | 2700 | G    |
| 1   | AS    | 2701 | U    |
| 1   | AS    | 2724 | U    |
| 1   | AS    | 2725 | G    |
| 1   | AS    | 2734 | A    |
| 1   | AS    | 2745 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 2749 | G    |
| 1   | AS    | 2750 | G    |
| 1   | AS    | 2768 | G    |
| 1   | AS    | 2771 | A    |
| 1   | AS    | 2772 | G    |
| 1   | AS    | 2773 | A    |
| 1   | AS    | 2774 | A    |
| 1   | AS    | 2782 | C    |
| 1   | AS    | 2786 | G    |
| 1   | AS    | 2789 | A    |
| 1   | AS    | 2790 | U    |
| 1   | AS    | 2814 | U    |
| 1   | AS    | 2815 | U    |
| 1   | AS    | 2817 | A    |
| 1   | AS    | 2833 | U    |
| 1   | AS    | 2839 | C    |
| 1   | AS    | 2843 | G    |
| 1   | AS    | 2844 | A    |
| 1   | AS    | 2847 | U    |
| 1   | AS    | 2859 | A    |
| 1   | AS    | 2861 | C    |
| 1   | AS    | 2866 | C    |
| 1   | AS    | 2870 | G    |
| 1   | AS    | 2871 | C    |
| 1   | AS    | 2886 | G    |
| 1   | AS    | 2895 | U    |
| 1   | AS    | 2907 | U    |
| 1   | AS    | 2908 | A    |
| 1   | AS    | 2911 | G    |
| 1   | AS    | 2914 | C    |
| 1   | AS    | 2919 | G    |
| 1   | AS    | 2920 | C    |
| 1   | AS    | 2923 | G    |
| 1   | AS    | 2926 | U    |
| 1   | AS    | 2943 | A    |
| 1   | AS    | 2955 | C    |
| 1   | AS    | 2960 | C    |
| 1   | AS    | 2962 | G    |
| 1   | AS    | 2969 | G    |
| 1   | AS    | 2984 | A    |
| 1   | AS    | 3021 | A    |
| 1   | AS    | 3028 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 3031 | G    |
| 1   | AS    | 3050 | A    |
| 1   | AS    | 3051 | C    |
| 1   | AS    | 3052 | G    |
| 1   | AS    | 3058 | A    |
| 1   | AS    | 3064 | C    |
| 1   | AS    | 3076 | U    |
| 1   | AS    | 3094 | A    |
| 1   | AS    | 3101 | A    |
| 1   | AS    | 3102 | A    |
| 1   | AS    | 3103 | U    |
| 1   | AS    | 3114 | A    |
| 1   | AS    | 3115 | C    |
| 1   | AS    | 3134 | C    |
| 1   | AS    | 3143 | G    |
| 1   | AS    | 3144 | A    |
| 1   | AS    | 3146 | G    |
| 1   | AS    | 3149 | U    |
| 1   | AS    | 3151 | C    |
| 1   | AS    | 3157 | A    |
| 1   | AS    | 3160 | C    |
| 1   | AS    | 3161 | U    |
| 1   | AS    | 3163 | U    |
| 1   | AS    | 3164 | U    |
| 1   | AS    | 3166 | A    |
| 1   | AS    | 3167 | G    |
| 1   | AS    | 3171 | C    |
| 1   | AS    | 3172 | U    |
| 1   | AS    | 3182 | C    |
| 1   | AS    | 3183 | A    |
| 1   | AS    | 3184 | G    |
| 1   | AS    | 3194 | G    |
| 1   | AS    | 3208 | A    |
| 1   | AS    | 3210 | A    |
| 1   | AS    | 3212 | G    |
| 1   | AS    | 3214 | U    |
| 1   | AS    | 3224 | U    |
| 1   | AS    | 3228 | G    |
| 1   | AS    | 3235 | A    |
| 1   | AS    | 3241 | G    |
| 1   | AS    | 3246 | C    |
| 1   | AS    | 3252 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 3259 | A    |
| 1   | AS    | 3260 | A    |
| 1   | AS    | 3268 | G    |
| 1   | AS    | 3269 | C    |
| 1   | AS    | 3272 | A    |
| 1   | AS    | 3278 | U    |
| 1   | AS    | 3281 | A    |
| 1   | AS    | 3284 | U    |
| 1   | AS    | 3285 | A    |
| 1   | AS    | 3306 | U    |
| 1   | AS    | 3307 | A    |
| 1   | AS    | 3309 | A    |
| 1   | AS    | 3310 | G    |
| 1   | AS    | 3316 | U    |
| 1   | AS    | 3317 | U    |
| 1   | AS    | 3318 | G    |
| 1   | AS    | 3319 | U    |
| 1   | AS    | 3320 | U    |
| 1   | AS    | 3321 | G    |
| 1   | AS    | 3334 | G    |
| 1   | AS    | 3343 | C    |
| 1   | AS    | 3351 | G    |
| 1   | AS    | 3361 | U    |
| 2   | AT    | 7    | G    |
| 2   | AT    | 22   | A    |
| 2   | AT    | 54   | U    |
| 2   | AT    | 55   | A    |
| 2   | AT    | 65   | G    |
| 2   | AT    | 73   | C    |
| 2   | AT    | 76   | A    |
| 2   | AT    | 102  | A    |
| 2   | AT    | 112  | G    |
| 3   | AU    | 23   | U    |
| 3   | AU    | 34   | U    |
| 3   | AU    | 35   | C    |
| 3   | AU    | 59   | A    |
| 3   | AU    | 62   | C    |
| 3   | AU    | 63   | G    |
| 3   | AU    | 81   | A    |
| 3   | AU    | 84   | C    |
| 3   | AU    | 85   | G    |
| 3   | AU    | 86   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AU    | 87  | G    |
| 3   | AU    | 92  | A    |
| 3   | AU    | 95  | G    |
| 3   | AU    | 102 | U    |
| 3   | AU    | 104 | A    |
| 3   | AU    | 105 | A    |
| 3   | AU    | 106 | C    |
| 3   | AU    | 111 | A    |
| 3   | AU    | 113 | U    |
| 3   | AU    | 125 | U    |
| 3   | AU    | 126 | A    |
| 3   | AU    | 152 | G    |
| 3   | AU    | 157 | U    |
| 46  | CM    | 17  | C    |
| 46  | CM    | 25  | C    |
| 46  | CM    | 26  | A    |
| 46  | CM    | 27  | U    |
| 46  | CM    | 34  | G    |
| 46  | CM    | 47  | A    |
| 46  | CM    | 57  | G    |
| 46  | CM    | 66  | U    |
| 46  | CM    | 72  | A    |
| 46  | CM    | 73  | U    |
| 46  | CM    | 74  | U    |
| 46  | CM    | 75  | U    |
| 46  | CM    | 76  | A    |
| 46  | CM    | 78  | A    |
| 46  | CM    | 79  | C    |
| 46  | CM    | 81  | G    |
| 46  | CM    | 84  | A    |
| 46  | CM    | 104 | A    |
| 46  | CM    | 114 | C    |
| 46  | CM    | 115 | G    |
| 46  | CM    | 123 | G    |
| 46  | CM    | 126 | A    |
| 46  | CM    | 127 | G    |
| 46  | CM    | 128 | U    |
| 46  | CM    | 138 | C    |
| 46  | CM    | 139 | U    |
| 46  | CM    | 142 | G    |
| 46  | CM    | 143 | A    |
| 46  | CM    | 150 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | CM    | 151 | G    |
| 46  | CM    | 152 | G    |
| 46  | CM    | 154 | A    |
| 46  | CM    | 159 | U    |
| 46  | CM    | 166 | A    |
| 46  | CM    | 168 | U    |
| 46  | CM    | 173 | G    |
| 46  | CM    | 176 | U    |
| 46  | CM    | 177 | A    |
| 46  | CM    | 190 | U    |
| 46  | CM    | 193 | G    |
| 46  | CM    | 199 | G    |
| 46  | CM    | 200 | A    |
| 46  | CM    | 202 | G    |
| 46  | CM    | 206 | U    |
| 46  | CM    | 211 | A    |
| 46  | CM    | 214 | U    |
| 46  | CM    | 215 | A    |
| 46  | CM    | 216 | A    |
| 46  | CM    | 217 | A    |
| 46  | CM    | 219 | A    |
| 46  | CM    | 220 | A    |
| 46  | CM    | 221 | U    |
| 46  | CM    | 222 | C    |
| 46  | CM    | 224 | A    |
| 46  | CM    | 225 | U    |
| 46  | CM    | 226 | G    |
| 46  | CM    | 228 | C    |
| 46  | CM    | 229 | U    |
| 46  | CM    | 230 | U    |
| 46  | CM    | 231 | C    |
| 46  | CM    | 234 | G    |
| 46  | CM    | 235 | C    |
| 46  | CM    | 236 | U    |
| 46  | CM    | 237 | C    |
| 46  | CM    | 238 | U    |
| 46  | CM    | 239 | U    |
| 46  | CM    | 240 | U    |
| 46  | CM    | 247 | U    |
| 46  | CM    | 255 | A    |
| 46  | CM    | 259 | U    |
| 46  | CM    | 260 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | CM    | 261 | C    |
| 46  | CM    | 262 | G    |
| 46  | CM    | 266 | C    |
| 46  | CM    | 269 | A    |
| 46  | CM    | 270 | U    |
| 46  | CM    | 274 | C    |
| 46  | CM    | 276 | U    |
| 46  | CM    | 277 | G    |
| 46  | CM    | 278 | U    |
| 46  | CM    | 279 | G    |
| 46  | CM    | 283 | G    |
| 46  | CM    | 285 | G    |
| 46  | CM    | 297 | A    |
| 46  | CM    | 312 | C    |
| 46  | CM    | 314 | A    |
| 46  | CM    | 318 | U    |
| 46  | CM    | 319 | C    |
| 46  | CM    | 320 | G    |
| 46  | CM    | 335 | G    |
| 46  | CM    | 336 | C    |
| 46  | CM    | 350 | A    |
| 46  | CM    | 357 | A    |
| 46  | CM    | 358 | A    |
| 46  | CM    | 359 | C    |
| 46  | CM    | 388 | G    |
| 46  | CM    | 398 | A    |
| 46  | CM    | 400 | C    |
| 46  | CM    | 402 | G    |
| 46  | CM    | 414 | A    |
| 46  | CM    | 416 | G    |
| 46  | CM    | 421 | G    |
| 46  | CM    | 422 | C    |
| 46  | CM    | 423 | A    |
| 46  | CM    | 424 | G    |
| 46  | CM    | 432 | G    |
| 46  | CM    | 437 | U    |
| 46  | CM    | 442 | C    |
| 46  | CM    | 446 | C    |
| 46  | CM    | 452 | A    |
| 46  | CM    | 458 | A    |
| 46  | CM    | 462 | A    |
| 46  | CM    | 466 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | CM    | 475 | A    |
| 46  | CM    | 480 | U    |
| 46  | CM    | 489 | C    |
| 46  | CM    | 490 | U    |
| 46  | CM    | 491 | U    |
| 46  | CM    | 495 | G    |
| 46  | CM    | 498 | C    |
| 46  | CM    | 499 | U    |
| 46  | CM    | 503 | A    |
| 46  | CM    | 504 | A    |
| 46  | CM    | 505 | U    |
| 46  | CM    | 506 | U    |
| 46  | CM    | 509 | A    |
| 46  | CM    | 512 | G    |
| 46  | CM    | 513 | A    |
| 46  | CM    | 515 | U    |
| 46  | CM    | 518 | A    |
| 46  | CM    | 519 | A    |
| 46  | CM    | 525 | A    |
| 46  | CM    | 530 | U    |
| 46  | CM    | 534 | C    |
| 46  | CM    | 536 | A    |
| 46  | CM    | 537 | G    |
| 46  | CM    | 539 | A    |
| 46  | CM    | 540 | A    |
| 46  | CM    | 547 | G    |
| 46  | CM    | 553 | A    |
| 46  | CM    | 554 | A    |
| 46  | CM    | 555 | G    |
| 46  | CM    | 556 | U    |
| 46  | CM    | 557 | C    |
| 46  | CM    | 563 | C    |
| 46  | CM    | 566 | G    |
| 46  | CM    | 576 | U    |
| 46  | CM    | 592 | A    |
| 46  | CM    | 593 | G    |
| 46  | CM    | 604 | A    |
| 46  | CM    | 609 | U    |
| 46  | CM    | 617 | A    |
| 46  | CM    | 618 | A    |
| 46  | CM    | 620 | A    |
| 46  | CM    | 621 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | CM    | 633 | A    |
| 46  | CM    | 639 | G    |
| 46  | CM    | 645 | G    |
| 46  | CM    | 648 | U    |
| 46  | CM    | 649 | G    |
| 46  | CM    | 650 | G    |
| 46  | CM    | 652 | C    |
| 46  | CM    | 653 | G    |
| 46  | CM    | 654 | G    |
| 46  | CM    | 655 | U    |
| 46  | CM    | 658 | A    |
| 46  | CM    | 659 | U    |
| 46  | CM    | 668 | U    |
| 46  | CM    | 669 | G    |
| 46  | CM    | 670 | C    |
| 46  | CM    | 671 | G    |
| 46  | CM    | 672 | U    |
| 46  | CM    | 673 | A    |
| 46  | CM    | 674 | C    |
| 46  | CM    | 675 | U    |
| 46  | CM    | 676 | G    |
| 46  | CM    | 678 | A    |
| 46  | CM    | 680 | C    |
| 46  | CM    | 681 | C    |
| 46  | CM    | 682 | A    |
| 46  | CM    | 688 | G    |
| 46  | CM    | 691 | U    |
| 46  | CM    | 694 | C    |
| 46  | CM    | 695 | C    |
| 46  | CM    | 696 | U    |
| 46  | CM    | 697 | U    |
| 46  | CM    | 700 | G    |
| 46  | CM    | 701 | G    |
| 46  | CM    | 702 | G    |
| 46  | CM    | 703 | U    |
| 46  | CM    | 719 | A    |
| 46  | CM    | 720 | C    |
| 46  | CM    | 722 | A    |
| 46  | CM    | 723 | G    |
| 46  | CM    | 724 | G    |
| 46  | CM    | 729 | U    |
| 46  | CM    | 739 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | CM    | 740 | A    |
| 46  | CM    | 741 | A    |
| 46  | CM    | 750 | G    |
| 46  | CM    | 751 | U    |
| 46  | CM    | 756 | A    |
| 46  | CM    | 759 | A    |
| 46  | CM    | 760 | G    |
| 46  | CM    | 762 | C    |
| 46  | CM    | 764 | U    |
| 46  | CM    | 765 | U    |
| 46  | CM    | 766 | U    |
| 46  | CM    | 767 | G    |
| 46  | CM    | 768 | C    |
| 46  | CM    | 770 | C    |
| 46  | CM    | 771 | G    |
| 46  | CM    | 773 | A    |
| 46  | CM    | 775 | A    |
| 46  | CM    | 778 | U    |
| 46  | CM    | 779 | U    |
| 46  | CM    | 796 | A    |
| 46  | CM    | 798 | A    |
| 46  | CM    | 799 | G    |
| 46  | CM    | 802 | C    |
| 46  | CM    | 803 | G    |
| 46  | CM    | 804 | U    |
| 46  | CM    | 805 | U    |
| 46  | CM    | 807 | U    |
| 46  | CM    | 808 | G    |
| 46  | CM    | 812 | C    |
| 46  | CM    | 813 | U    |
| 46  | CM    | 814 | A    |
| 46  | CM    | 815 | U    |
| 46  | CM    | 816 | U    |
| 46  | CM    | 818 | U    |
| 46  | CM    | 819 | G    |
| 46  | CM    | 820 | U    |
| 46  | CM    | 821 | U    |
| 46  | CM    | 823 | G    |
| 46  | CM    | 824 | U    |
| 46  | CM    | 825 | U    |
| 46  | CM    | 826 | U    |
| 46  | CM    | 827 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | CM    | 828  | U    |
| 46  | CM    | 829  | A    |
| 46  | CM    | 840  | A    |
| 46  | CM    | 842  | U    |
| 46  | CM    | 848  | A    |
| 46  | CM    | 856  | G    |
| 46  | CM    | 857  | G    |
| 46  | CM    | 869  | A    |
| 46  | CM    | 871  | U    |
| 46  | CM    | 875  | C    |
| 46  | CM    | 877  | G    |
| 46  | CM    | 878  | U    |
| 46  | CM    | 879  | U    |
| 46  | CM    | 881  | U    |
| 46  | CM    | 891  | A    |
| 46  | CM    | 909  | A    |
| 46  | CM    | 910  | G    |
| 46  | CM    | 911  | A    |
| 46  | CM    | 918  | A    |
| 46  | CM    | 920  | U    |
| 46  | CM    | 927  | G    |
| 46  | CM    | 945  | U    |
| 46  | CM    | 951  | A    |
| 46  | CM    | 973  | A    |
| 46  | CM    | 975  | C    |
| 46  | CM    | 977  | A    |
| 46  | CM    | 988  | A    |
| 46  | CM    | 989  | U    |
| 46  | CM    | 990  | A    |
| 46  | CM    | 997  | U    |
| 46  | CM    | 998  | A    |
| 46  | CM    | 1004 | A    |
| 46  | CM    | 1005 | A    |
| 46  | CM    | 1011 | A    |
| 46  | CM    | 1013 | C    |
| 46  | CM    | 1017 | G    |
| 46  | CM    | 1024 | A    |
| 46  | CM    | 1025 | G    |
| 46  | CM    | 1039 | U    |
| 46  | CM    | 1042 | U    |
| 46  | CM    | 1043 | U    |
| 46  | CM    | 1055 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | CM    | 1056 | U    |
| 46  | CM    | 1057 | C    |
| 46  | CM    | 1058 | G    |
| 46  | CM    | 1059 | G    |
| 46  | CM    | 1060 | C    |
| 46  | CM    | 1061 | A    |
| 46  | CM    | 1067 | C    |
| 46  | CM    | 1074 | U    |
| 46  | CM    | 1077 | A    |
| 46  | CM    | 1081 | C    |
| 46  | CM    | 1085 | G    |
| 46  | CM    | 1123 | A    |
| 46  | CM    | 1135 | G    |
| 46  | CM    | 1143 | C    |
| 46  | CM    | 1145 | A    |
| 46  | CM    | 1152 | G    |
| 46  | CM    | 1168 | A    |
| 46  | CM    | 1169 | A    |
| 46  | CM    | 1170 | U    |
| 46  | CM    | 1179 | A    |
| 46  | CM    | 1181 | A    |
| 46  | CM    | 1184 | G    |
| 46  | CM    | 1185 | G    |
| 46  | CM    | 1186 | G    |
| 46  | CM    | 1187 | A    |
| 46  | CM    | 1193 | A    |
| 46  | CM    | 1202 | A    |
| 46  | CM    | 1203 | G    |
| 46  | CM    | 1206 | A    |
| 46  | CM    | 1207 | C    |
| 46  | CM    | 1212 | A    |
| 46  | CM    | 1215 | A    |
| 46  | CM    | 1219 | A    |
| 46  | CM    | 1220 | C    |
| 46  | CM    | 1221 | A    |
| 46  | CM    | 1229 | A    |
| 46  | CM    | 1230 | G    |
| 46  | CM    | 1231 | C    |
| 46  | CM    | 1236 | U    |
| 46  | CM    | 1243 | U    |
| 46  | CM    | 1250 | G    |
| 46  | CM    | 1270 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | CM    | 1284 | G    |
| 46  | CM    | 1299 | U    |
| 46  | CM    | 1300 | U    |
| 46  | CM    | 1301 | G    |
| 46  | CM    | 1306 | A    |
| 46  | CM    | 1325 | U    |
| 46  | CM    | 1330 | A    |
| 46  | CM    | 1336 | G    |
| 46  | CM    | 1339 | G    |
| 46  | CM    | 1342 | A    |
| 46  | CM    | 1343 | G    |
| 46  | CM    | 1345 | A    |
| 46  | CM    | 1346 | U    |
| 46  | CM    | 1348 | U    |
| 46  | CM    | 1349 | G    |
| 46  | CM    | 1352 | G    |
| 46  | CM    | 1355 | A    |
| 46  | CM    | 1356 | U    |
| 46  | CM    | 1357 | A    |
| 46  | CM    | 1358 | G    |
| 46  | CM    | 1359 | U    |
| 46  | CM    | 1360 | C    |
| 46  | CM    | 1364 | U    |
| 46  | CM    | 1365 | C    |
| 46  | CM    | 1369 | G    |
| 46  | CM    | 1370 | A    |
| 46  | CM    | 1376 | U    |
| 46  | CM    | 1380 | G    |
| 46  | CM    | 1381 | A    |
| 46  | CM    | 1382 | U    |
| 46  | CM    | 1384 | U    |
| 46  | CM    | 1385 | C    |
| 46  | CM    | 1392 | A    |
| 46  | CM    | 1397 | A    |
| 46  | CM    | 1398 | G    |
| 46  | CM    | 1399 | U    |
| 46  | CM    | 1400 | U    |
| 46  | CM    | 1401 | U    |
| 46  | CM    | 1410 | A    |
| 46  | CM    | 1413 | A    |
| 46  | CM    | 1414 | G    |
| 46  | CM    | 1415 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | CM    | 1422 | A    |
| 46  | CM    | 1431 | G    |
| 46  | CM    | 1433 | C    |
| 46  | CM    | 1445 | C    |
| 46  | CM    | 1446 | A    |
| 46  | CM    | 1455 | A    |
| 46  | CM    | 1457 | A    |
| 46  | CM    | 1458 | C    |
| 46  | CM    | 1461 | A    |
| 46  | CM    | 1462 | C    |
| 46  | CM    | 1463 | G    |
| 46  | CM    | 1468 | C    |
| 46  | CM    | 1476 | A    |
| 46  | CM    | 1477 | U    |
| 46  | CM    | 1480 | G    |
| 46  | CM    | 1483 | U    |
| 46  | CM    | 1491 | G    |
| 46  | CM    | 1502 | A    |
| 46  | CM    | 1503 | A    |
| 46  | CM    | 1508 | G    |
| 46  | CM    | 1510 | G    |
| 46  | CM    | 1511 | A    |
| 46  | CM    | 1523 | G    |
| 46  | CM    | 1524 | C    |
| 46  | CM    | 1529 | G    |
| 46  | CM    | 1530 | A    |
| 46  | CM    | 1541 | U    |
| 46  | CM    | 1544 | U    |
| 46  | CM    | 1546 | G    |
| 46  | CM    | 1556 | A    |
| 46  | CM    | 1560 | A    |
| 46  | CM    | 1561 | G    |
| 46  | CM    | 1571 | G    |
| 46  | CM    | 1574 | A    |
| 46  | CM    | 1575 | G    |
| 46  | CM    | 1577 | G    |
| 46  | CM    | 1580 | A    |
| 46  | CM    | 1582 | U    |
| 46  | CM    | 1584 | A    |
| 46  | CM    | 1588 | G    |
| 46  | CM    | 1621 | C    |
| 46  | CM    | 1644 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | CM    | 1645 | G    |
| 46  | CM    | 1665 | C    |
| 46  | CM    | 1667 | G    |
| 46  | CM    | 1670 | U    |
| 46  | CM    | 1671 | G    |
| 46  | CM    | 1673 | U    |
| 46  | CM    | 1702 | A    |
| 46  | CM    | 1704 | C    |
| 46  | CM    | 1737 | A    |
| 46  | CM    | 1742 | A    |
| 46  | CM    | 1743 | A    |
| 46  | CM    | 1744 | G    |
| 46  | CM    | 1747 | G    |
| 46  | CM    | 1749 | A    |
| 46  | CM    | 1753 | A    |
| 46  | CM    | 1756 | U    |
| 46  | CM    | 1767 | G    |
| 46  | CM    | 1770 | C    |
| 46  | CM    | 1779 | G    |
| 46  | CM    | 1780 | G    |
| 46  | CM    | 1781 | A    |
| 46  | CM    | 1782 | U    |
| 46  | CM    | 1783 | C    |

All (182) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 172  | C    |
| 1   | 1     | 403  | C    |
| 1   | 1     | 538  | G    |
| 1   | 1     | 563  | U    |
| 1   | 1     | 601  | U    |
| 1   | 1     | 759  | G    |
| 1   | 1     | 912  | G    |
| 1   | 1     | 1011 | C    |
| 1   | 1     | 1012 | U    |
| 1   | 1     | 1029 | U    |
| 1   | 1     | 1060 | A    |
| 1   | 1     | 1099 | A    |
| 1   | 1     | 1346 | U    |
| 1   | 1     | 1347 | U    |
| 1   | 1     | 1559 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1561 | U    |
| 1   | 1     | 1576 | A    |
| 1   | 1     | 1762 | G    |
| 1   | 1     | 1815 | U    |
| 1   | 1     | 1943 | G    |
| 1   | 1     | 2090 | U    |
| 1   | 1     | 2182 | C    |
| 1   | 1     | 2183 | U    |
| 1   | 1     | 2441 | G    |
| 1   | 1     | 2442 | U    |
| 1   | 1     | 2443 | G    |
| 1   | 1     | 2447 | G    |
| 1   | 1     | 2455 | G    |
| 1   | 1     | 2465 | U    |
| 1   | 1     | 2476 | C    |
| 1   | 1     | 2515 | G    |
| 1   | 1     | 2519 | A    |
| 1   | 1     | 2545 | C    |
| 1   | 1     | 2789 | A    |
| 1   | 1     | 2790 | U    |
| 1   | 1     | 3093 | U    |
| 1   | 1     | 3163 | U    |
| 1   | 1     | 3164 | U    |
| 1   | 1     | 3165 | U    |
| 1   | 1     | 3193 | C    |
| 1   | 1     | 3234 | U    |
| 1   | 1     | 3240 | U    |
| 1   | 1     | 3284 | U    |
| 1   | 1     | 3309 | A    |
| 1   | 1     | 3317 | U    |
| 3   | 4     | 85   | G    |
| 3   | 4     | 125  | U    |
| 46  | B     | 25   | C    |
| 46  | B     | 78   | A    |
| 46  | B     | 137  | A    |
| 46  | B     | 151  | G    |
| 46  | B     | 176  | U    |
| 46  | B     | 215  | A    |
| 46  | B     | 216  | A    |
| 46  | B     | 235  | C    |
| 46  | B     | 259  | U    |
| 46  | B     | 265  | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | B     | 278  | U    |
| 46  | B     | 415  | A    |
| 46  | B     | 451  | C    |
| 46  | B     | 505  | U    |
| 46  | B     | 514  | G    |
| 46  | B     | 518  | A    |
| 46  | B     | 529  | C    |
| 46  | B     | 533  | A    |
| 46  | B     | 553  | A    |
| 46  | B     | 556  | U    |
| 46  | B     | 638  | U    |
| 46  | B     | 740  | A    |
| 46  | B     | 763  | C    |
| 46  | B     | 769  | U    |
| 46  | B     | 814  | A    |
| 46  | B     | 820  | U    |
| 46  | B     | 855  | C    |
| 46  | B     | 874  | U    |
| 46  | B     | 876  | A    |
| 46  | B     | 1168 | A    |
| 46  | B     | 1335 | U    |
| 46  | B     | 1355 | A    |
| 46  | B     | 1369 | G    |
| 46  | B     | 1396 | A    |
| 46  | B     | 1398 | G    |
| 46  | B     | 1457 | A    |
| 46  | B     | 1467 | C    |
| 46  | B     | 1479 | A    |
| 46  | B     | 1484 | U    |
| 46  | B     | 1523 | G    |
| 46  | B     | 1573 | A    |
| 46  | B     | 1579 | A    |
| 46  | B     | 1581 | G    |
| 46  | B     | 1703 | C    |
| 46  | B     | 1743 | A    |
| 1   | AS    | 172  | C    |
| 1   | AS    | 403  | C    |
| 1   | AS    | 447  | U    |
| 1   | AS    | 487  | C    |
| 1   | AS    | 538  | G    |
| 1   | AS    | 563  | U    |
| 1   | AS    | 601  | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AS    | 759  | G    |
| 1   | AS    | 912  | G    |
| 1   | AS    | 1029 | U    |
| 1   | AS    | 1060 | A    |
| 1   | AS    | 1099 | A    |
| 1   | AS    | 1346 | U    |
| 1   | AS    | 1347 | U    |
| 1   | AS    | 1559 | C    |
| 1   | AS    | 1576 | A    |
| 1   | AS    | 1762 | G    |
| 1   | AS    | 1815 | U    |
| 1   | AS    | 1943 | G    |
| 1   | AS    | 2090 | U    |
| 1   | AS    | 2182 | C    |
| 1   | AS    | 2183 | U    |
| 1   | AS    | 2430 | G    |
| 1   | AS    | 2515 | G    |
| 1   | AS    | 2519 | A    |
| 1   | AS    | 2545 | C    |
| 1   | AS    | 2667 | A    |
| 1   | AS    | 2789 | A    |
| 1   | AS    | 2790 | U    |
| 1   | AS    | 3093 | U    |
| 1   | AS    | 3159 | A    |
| 1   | AS    | 3160 | C    |
| 1   | AS    | 3193 | C    |
| 1   | AS    | 3234 | U    |
| 1   | AS    | 3240 | U    |
| 1   | AS    | 3284 | U    |
| 1   | AS    | 3309 | A    |
| 1   | AS    | 3315 | C    |
| 1   | AS    | 3317 | U    |
| 3   | AU    | 85   | G    |
| 3   | AU    | 125  | U    |
| 3   | AU    | 156  | U    |
| 46  | CM    | 25   | C    |
| 46  | CM    | 65   | A    |
| 46  | CM    | 74   | U    |
| 46  | CM    | 78   | A    |
| 46  | CM    | 137  | A    |
| 46  | CM    | 151  | G    |
| 46  | CM    | 176  | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 46  | CM    | 214  | U    |
| 46  | CM    | 237  | C    |
| 46  | CM    | 259  | U    |
| 46  | CM    | 265  | U    |
| 46  | CM    | 415  | A    |
| 46  | CM    | 451  | C    |
| 46  | CM    | 504  | A    |
| 46  | CM    | 505  | U    |
| 46  | CM    | 514  | G    |
| 46  | CM    | 518  | A    |
| 46  | CM    | 529  | C    |
| 46  | CM    | 533  | A    |
| 46  | CM    | 553  | A    |
| 46  | CM    | 556  | U    |
| 46  | CM    | 638  | U    |
| 46  | CM    | 680  | C    |
| 46  | CM    | 690  | C    |
| 46  | CM    | 695  | C    |
| 46  | CM    | 740  | A    |
| 46  | CM    | 763  | C    |
| 46  | CM    | 769  | U    |
| 46  | CM    | 814  | A    |
| 46  | CM    | 817  | U    |
| 46  | CM    | 855  | C    |
| 46  | CM    | 874  | U    |
| 46  | CM    | 876  | A    |
| 46  | CM    | 1168 | A    |
| 46  | CM    | 1335 | U    |
| 46  | CM    | 1359 | U    |
| 46  | CM    | 1369 | G    |
| 46  | CM    | 1396 | A    |
| 46  | CM    | 1398 | G    |
| 46  | CM    | 1457 | A    |
| 46  | CM    | 1467 | C    |
| 46  | CM    | 1479 | A    |
| 46  | CM    | 1523 | G    |
| 46  | CM    | 1555 | C    |
| 46  | CM    | 1573 | A    |
| 46  | CM    | 1579 | A    |
| 46  | CM    | 1581 | G    |
| 46  | CM    | 1742 | A    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1152 ligands modelled in this entry, 1148 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 83  | 3K5  | AS    | 3401 | -    | 63,63,63     | 0.35 | 0           | 84,95,95    | 0.91 | 3 (3%)      |
| 86  | GET  | B     | 1851 | -    | 35,36,36     | 0.44 | 0           | 43,55,55    | 0.63 | 1 (2%)      |
| 83  | 3K5  | 1     | 3401 | -    | 63,63,63     | 0.26 | 0           | 84,95,95    | 0.46 | 1 (1%)      |
| 86  | GET  | CM    | 1822 | -    | 35,36,36     | 0.44 | 0           | 43,55,55    | 0.66 | 1 (2%)      |

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   |
|-----|------|-------|------|------|---------|--------------|---------|
| 83  | 3K5  | AS    | 3401 | -    | -       | 4/29/121/121 | 0/7/7/7 |
| 86  | GET  | B     | 1851 | -    | -       | 5/13/74/74   | 0/3/3/3 |
| 83  | 3K5  | 1     | 3401 | -    | -       | 4/29/121/121 | 0/7/7/7 |
| 86  | GET  | CM    | 1822 | -    | -       | 2/13/74/74   | 0/3/3/3 |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 83  | AS    | 3401 | 3K5  | C34-O14-C38 | 4.25 | 124.32      | 117.72   |
| 83  | AS    | 3401 | 3K5  | O14-C34-C35 | 3.90 | 116.71      | 107.76   |
| 86  | CM    | 1822 | GET  | O11-C11-C21 | 3.44 | 113.70      | 108.08   |
| 83  | AS    | 3401 | 3K5  | O14-C34-C33 | 3.37 | 115.51      | 107.76   |
| 86  | B     | 1851 | GET  | O11-C11-C21 | 2.81 | 112.67      | 108.08   |
| 83  | 1     | 3401 | 3K5  | O1-C5-C1    | 2.25 | 110.42      | 107.23   |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 86  | B     | 1851 | GET  | O51-C51-C61-O61 |
| 86  | B     | 1851 | GET  | C23-C33-N33-C93 |
| 83  | 1     | 3401 | 3K5  | C39-C38-O14-C34 |
| 83  | 1     | 3401 | 3K5  | C31-C30-O9-C26  |
| 83  | 1     | 3401 | 3K5  | O15-C38-O14-C34 |
| 83  | 1     | 3401 | 3K5  | O10-C30-O9-C26  |
| 83  | AS    | 3401 | 3K5  | O15-C38-O14-C34 |
| 83  | AS    | 3401 | 3K5  | C39-C38-O14-C34 |
| 83  | AS    | 3401 | 3K5  | C33-C34-O14-C38 |
| 86  | CM    | 1822 | GET  | O51-C11-O11-C42 |
| 86  | CM    | 1822 | GET  | C23-C33-N33-C93 |
| 83  | AS    | 3401 | 3K5  | O7-C24-O6-C23   |
| 86  | B     | 1851 | GET  | O51-C51-C61-C71 |
| 86  | B     | 1851 | GET  | C41-C51-C61-C71 |
| 86  | B     | 1851 | GET  | C52-C42-O11-C11 |

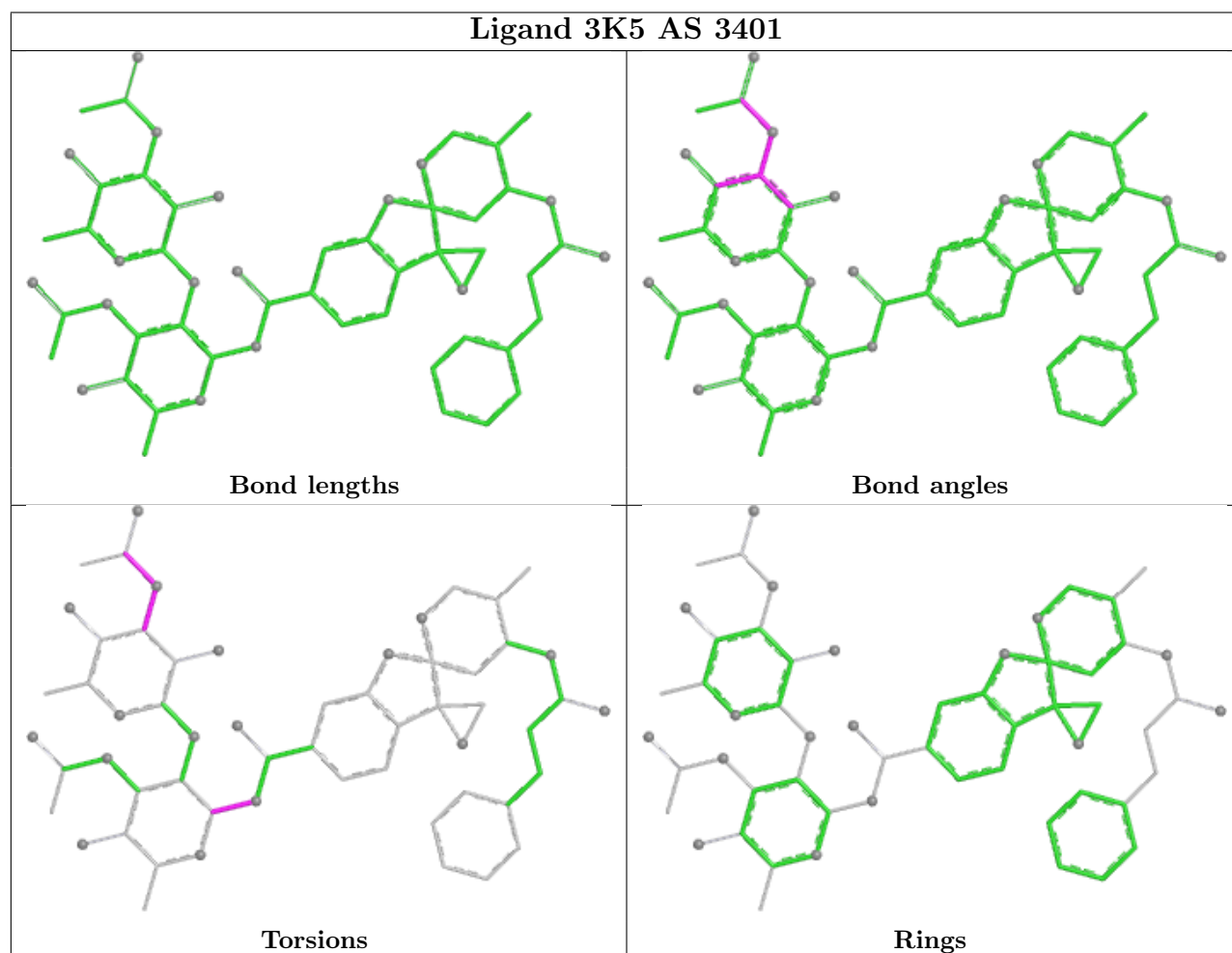
There are no ring outliers.

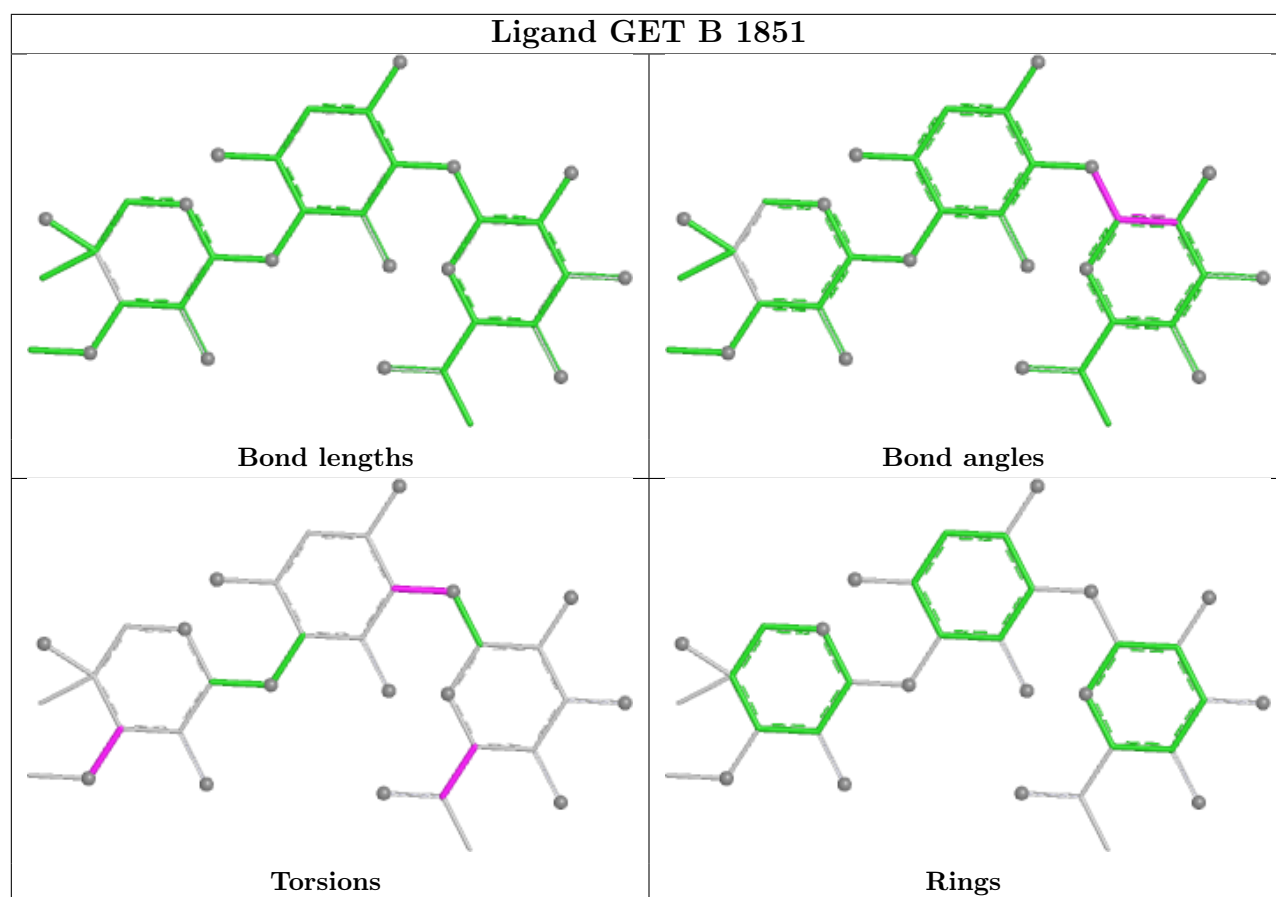
4 monomers are involved in 24 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 83  | AS    | 3401 | 3K5  | 7       | 0            |
| 86  | B     | 1851 | GET  | 6       | 0            |
| 83  | 1     | 3401 | 3K5  | 6       | 0            |
| 86  | CM    | 1822 | GET  | 5       | 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

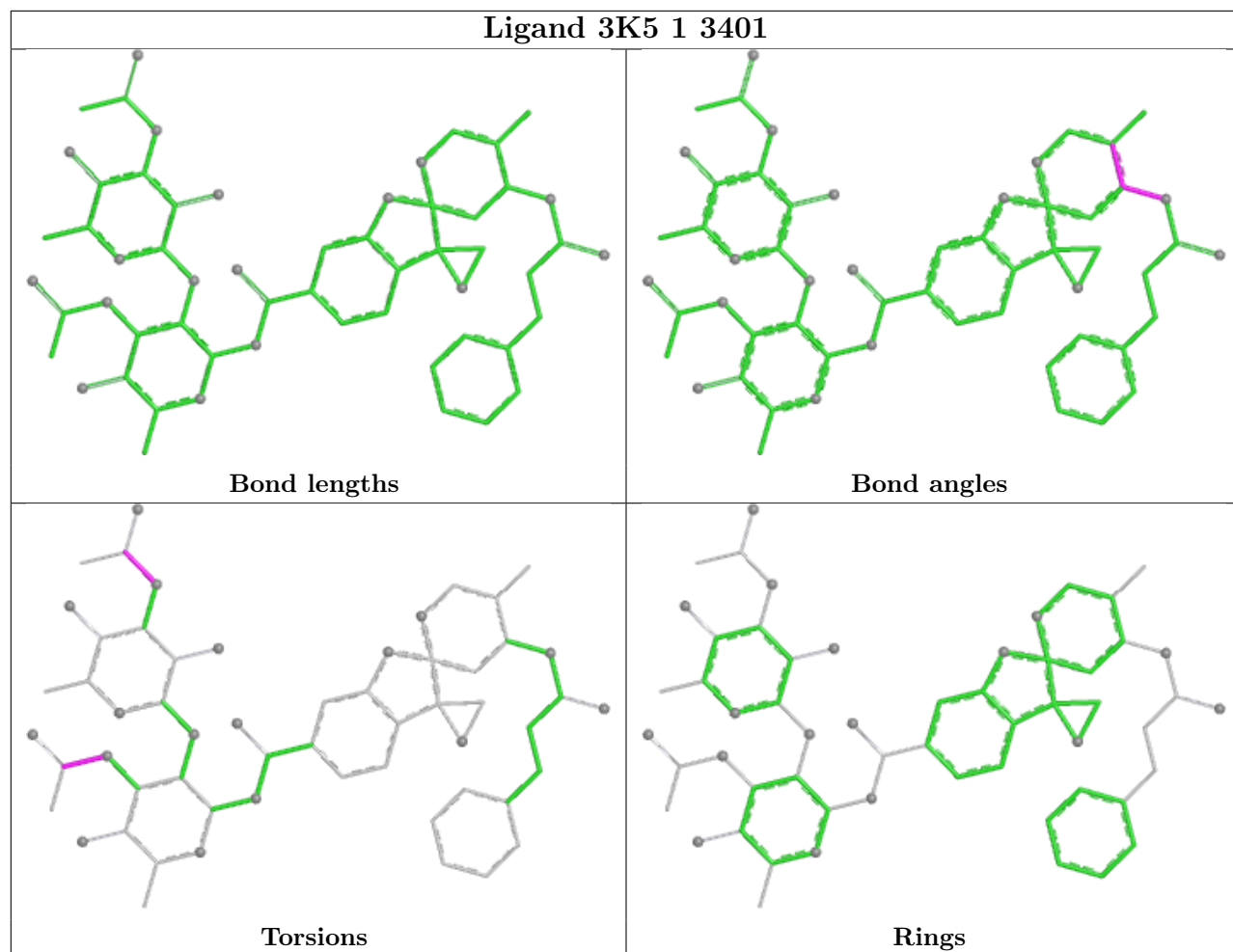
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

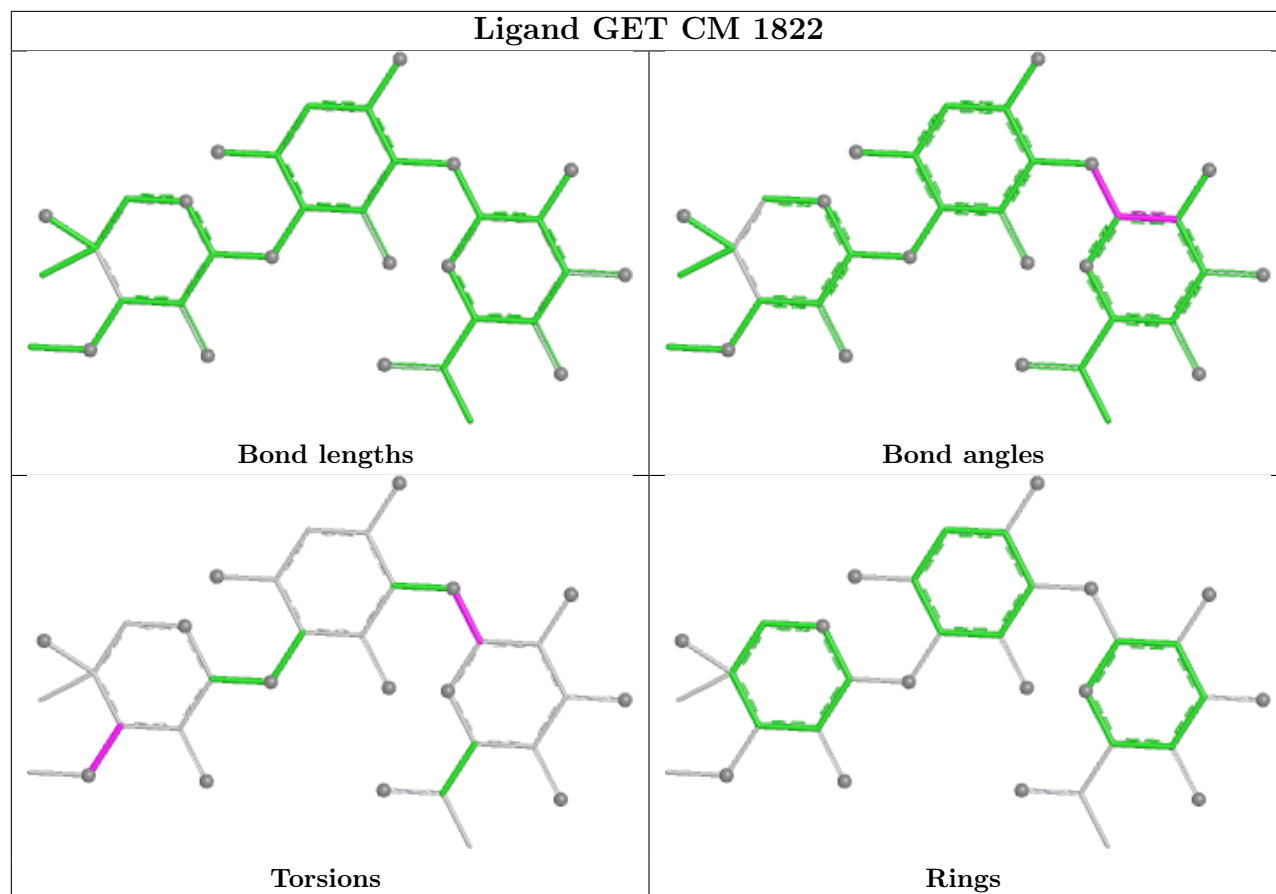






## Ligand 3K5 1 3401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 1   | 1     | 3218/3359 (95%) | 0.17   | 104 (3%) | 50 | 29 | 67, 107, 226, 432     | 0     |
| 1   | AS    | 3101/3359 (92%) | 0.29   | 142 (4%) | 37 | 20 | 74, 119, 222, 327     | 0     |
| 2   | 3     | 121/121 (100%)  | -0.11  | 2 (1%)   | 69 | 43 | 81, 112, 128, 178     | 0     |
| 2   | AT    | 121/121 (100%)  | 0.03   | 1 (0%)   | 82 | 60 | 86, 122, 141, 189     | 0     |
| 3   | 4     | 156/158 (98%)   | 0.08   | 4 (2%)   | 57 | 33 | 88, 119, 158, 213     | 0     |
| 3   | AU    | 158/158 (100%)  | 0.26   | 7 (4%)   | 39 | 21 | 103, 142, 189, 269    | 0     |
| 4   | AW    | 249/254 (98%)   | 0.51   | 24 (9%)  | 13 | 9  | 88, 128, 152, 164     | 0     |
| 4   | j     | 249/254 (98%)   | 0.50   | 16 (6%)  | 25 | 15 | 67, 103, 134, 178     | 0     |
| 5   | AX    | 386/389 (99%)   | 0.43   | 29 (7%)  | 20 | 13 | 61, 100, 137, 204     | 0     |
| 5   | k     | 386/389 (99%)   | 0.42   | 22 (5%)  | 29 | 17 | 59, 100, 127, 167     | 0     |
| 6   | AY    | 359/363 (98%)   | 0.70   | 47 (13%) | 7  | 6  | 76, 125, 157, 177     | 0     |
| 6   | l     | 359/363 (98%)   | 0.58   | 25 (6%)  | 22 | 14 | 58, 111, 144, 177     | 0     |
| 7   | AZ    | 292/298 (97%)   | 0.70   | 29 (9%)  | 13 | 8  | 88, 141, 175, 185     | 0     |
| 7   | m     | 294/298 (98%)   | 0.28   | 23 (7%)  | 19 | 12 | 88, 123, 160, 181     | 0     |
| 8   | BA    | 153/176 (86%)   | 0.64   | 15 (9%)  | 13 | 9  | 92, 129, 157, 192     | 0     |
| 8   | n     | 157/176 (89%)   | 0.32   | 6 (3%)   | 44 | 24 | 93, 124, 156, 186     | 0     |
| 9   | BB    | 226/241 (93%)   | 0.54   | 24 (10%) | 11 | 8  | 75, 107, 144, 180     | 0     |
| 9   | o     | 229/241 (95%)   | 0.26   | 12 (5%)  | 33 | 19 | 70, 97, 140, 210      | 0     |
| 10  | BC    | 233/262 (88%)   | 0.30   | 9 (3%)   | 43 | 23 | 132, 169, 208, 223    | 0     |
| 10  | p     | 236/262 (90%)   | 0.21   | 8 (3%)   | 48 | 27 | 101, 134, 180, 207    | 0     |
| 11  | BD    | 190/191 (99%)   | 0.23   | 10 (5%)  | 32 | 18 | 97, 127, 155, 192     | 0     |
| 11  | q     | 190/191 (99%)   | 0.17   | 1 (0%)   | 87 | 68 | 84, 115, 139, 174     | 0     |
| 12  | r     | 207/219 (94%)   | 0.23   | 7 (3%)   | 48 | 27 | 57, 93, 137, 168      | 0     |
| 13  | BF    | 171/174 (98%)   | 0.24   | 7 (4%)   | 41 | 22 | 91, 132, 162, 183     | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 13  | s     | 171/174 (98%) | 0.33   | 10 (5%) 29 17 | 82, 126, 154, 168     | 0     |
| 14  | BG    | 200/202 (99%) | 0.30   | 8 (4%) 42 23  | 88, 140, 182, 202     | 0     |
| 14  | t     | 200/202 (99%) | 0.20   | 11 (5%) 30 18 | 68, 122, 169, 194     | 0     |
| 15  | BH    | 130/131 (99%) | 0.23   | 3 (2%) 61 37  | 90, 123, 153, 167     | 0     |
| 15  | u     | 128/131 (97%) | 0.23   | 9 (7%) 22 14  | 87, 112, 136, 151     | 0     |
| 16  | BI    | 203/204 (99%) | 1.21   | 34 (16%) 4 4  | 93, 134, 156, 171     | 0     |
| 16  | v     | 203/204 (99%) | 1.03   | 36 (17%) 4 4  | 74, 104, 123, 140     | 0     |
| 17  | BJ    | 199/200 (99%) | 0.43   | 14 (7%) 22 14 | 74, 100, 145, 164     | 0     |
| 17  | w     | 199/200 (99%) | 0.44   | 10 (5%) 34 19 | 69, 96, 136, 157      | 0     |
| 18  | BK    | 174/185 (94%) | 0.50   | 7 (4%) 42 23  | 82, 114, 142, 165     | 0     |
| 18  | x     | 169/185 (91%) | 0.57   | 9 (5%) 32 18  | 75, 105, 153, 171     | 0     |
| 19  | BL    | 185/186 (99%) | 0.73   | 17 (9%) 14 9  | 91, 120, 141, 159     | 0     |
| 19  | y     | 185/186 (99%) | 0.55   | 16 (8%) 16 11 | 75, 106, 131, 150     | 0     |
| 20  | BM    | 179/190 (94%) | 0.47   | 14 (7%) 19 12 | 103, 134, 198, 217    | 0     |
| 20  | z     | 179/190 (94%) | 0.61   | 14 (7%) 19 12 | 91, 120, 185, 204     | 0     |
| 21  | 0     | 170/172 (98%) | 0.16   | 3 (1%) 67 42  | 75, 96, 124, 174      | 0     |
| 21  | BN    | 170/172 (98%) | 0.21   | 0 100 100     | 81, 110, 135, 159     | 0     |
| 22  | 2     | 159/160 (99%) | 0.41   | 11 (6%) 23 14 | 74, 97, 165, 186      | 0     |
| 22  | BO    | 159/160 (99%) | 0.74   | 16 (10%) 12 8 | 80, 109, 165, 203     | 0     |
| 23  | 5     | 100/124 (80%) | 0.02   | 0 100 100     | 122, 159, 188, 195    | 0     |
| 23  | BP    | 99/124 (79%)  | -0.23  | 0 100 100     | 137, 175, 196, 243    | 0     |
| 24  | 6     | 131/137 (95%) | 0.57   | 8 (6%) 27 16  | 69, 92, 121, 137      | 0     |
| 24  | BQ    | 131/137 (95%) | 0.45   | 5 (3%) 44 24  | 58, 94, 121, 142      | 0     |
| 25  | 7     | 118/155 (76%) | 0.03   | 0 100 100     | 80, 126, 175, 186     | 0     |
| 25  | BR    | 109/155 (70%) | 0.20   | 5 (4%) 37 20  | 84, 117, 150, 174     | 0     |
| 26  | 8     | 120/142 (84%) | 0.48   | 13 (10%) 11 8 | 93, 123, 143, 156     | 0     |
| 26  | BS    | 119/142 (83%) | 0.38   | 6 (5%) 34 19  | 118, 146, 163, 176    | 0     |
| 27  | 9     | 126/127 (99%) | 0.32   | 2 (1%) 70 45  | 92, 126, 155, 164     | 0     |
| 27  | BT    | 126/127 (99%) | 0.45   | 7 (5%) 30 17  | 110, 143, 174, 191    | 0     |
| 28  | AA    | 135/136 (99%) | 0.25   | 4 (2%) 52 30  | 112, 141, 166, 198    | 0     |
| 28  | BU    | 135/136 (99%) | 0.03   | 1 (0%) 84 63  | 138, 171, 197, 224    | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2  |         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------|---------|-----------------------|-------|
| 29  | AB    | 148/149 (99%) | 0.66   | 13 (8%)  | 15 10   | 70, 101, 132, 161     | 0     |
| 29  | BV    | 148/149 (99%) | 0.67   | 11 (7%)  | 20 13   | 77, 124, 153, 170     | 0     |
| 30  | AC    | 58/63 (92%)   | 0.69   | 10 (17%) | 4 4     | 69, 114, 142, 164     | 0     |
| 30  | BW    | 60/63 (95%)   | 0.96   | 11 (18%) | 3 4     | 87, 130, 167, 194     | 0     |
| 31  | AD    | 98/106 (92%)  | 0.16   | 0        | 100 100 | 99, 130, 149, 153     | 0     |
| 31  | BX    | 94/106 (88%)  | -0.01  | 0        | 100 100 | 129, 160, 181, 199    | 0     |
| 32  | AE    | 108/112 (96%) | 0.33   | 7 (6%)   | 25 15   | 86, 115, 163, 184     | 0     |
| 32  | BY    | 108/112 (96%) | 0.52   | 9 (8%)   | 17 11   | 87, 120, 164, 203     | 0     |
| 33  | AF    | 124/131 (94%) | 0.84   | 15 (12%) | 8 6     | 64, 105, 131, 151     | 0     |
| 33  | BZ    | 122/131 (93%) | 0.85   | 11 (9%)  | 15 10   | 88, 112, 140, 154     | 0     |
| 34  | AG    | 106/107 (99%) | 0.51   | 8 (7%)   | 20 13   | 76, 102, 120, 142     | 0     |
| 34  | CA    | 106/107 (99%) | 0.29   | 1 (0%)   | 81 58   | 85, 106, 127, 144     | 0     |
| 35  | AH    | 112/122 (91%) | 1.08   | 25 (22%) | 2 2     | 87, 121, 168, 190     | 0     |
| 35  | CB    | 110/122 (90%) | 1.10   | 21 (19%) | 3 3     | 112, 146, 194, 201    | 0     |
| 36  | AI    | 115/120 (95%) | 0.33   | 6 (5%)   | 33 19   | 105, 131, 157, 175    | 0     |
| 36  | CC    | 117/120 (97%) | 0.45   | 7 (5%)   | 27 16   | 127, 155, 175, 210    | 0     |
| 37  | AJ    | 97/99 (97%)   | 0.10   | 2 (2%)   | 63 38   | 103, 119, 155, 199    | 0     |
| 37  | CD    | 95/99 (95%)   | 0.20   | 2 (2%)   | 63 38   | 115, 148, 174, 197    | 0     |
| 38  | AK    | 86/90 (95%)   | 0.62   | 6 (6%)   | 22 14   | 81, 102, 141, 152     | 0     |
| 38  | CE    | 86/90 (95%)   | 0.60   | 6 (6%)   | 22 14   | 88, 120, 160, 169     | 0     |
| 39  | AL    | 77/78 (98%)   | 0.38   | 1 (1%)   | 75 50   | 113, 152, 178, 207    | 0     |
| 39  | CF    | 77/78 (98%)   | 0.04   | 2 (2%)   | 57 33   | 140, 167, 202, 208    | 0     |
| 40  | AM    | 50/51 (98%)   | 0.68   | 3 (6%)   | 27 16   | 84, 111, 135, 143     | 0     |
| 40  | CG    | 50/51 (98%)   | 0.72   | 5 (10%)  | 12 8    | 95, 125, 143, 147     | 0     |
| 41  | AN    | 50/52 (96%)   | 0.85   | 5 (10%)  | 12 8    | 113, 149, 165, 169    | 0     |
| 41  | CH    | 50/52 (96%)   | 0.95   | 7 (14%)  | 6 5     | 121, 154, 169, 181    | 0     |
| 42  | AO    | 25/25 (100%)  | 1.15   | 4 (16%)  | 5 4     | 99, 107, 123, 130     | 0     |
| 42  | CI    | 24/25 (96%)   | 1.18   | 4 (16%)  | 4 4     | 93, 112, 125, 132     | 0     |
| 43  | AP    | 103/106 (97%) | 0.22   | 2 (1%)   | 66 41   | 73, 100, 143, 158     | 0     |
| 43  | CJ    | 103/106 (97%) | 0.42   | 6 (5%)   | 29 17   | 91, 124, 160, 171     | 0     |
| 44  | AQ    | 91/92 (98%)   | 0.44   | 5 (5%)   | 30 18   | 79, 111, 140, 165     | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 44  | CK    | 91/92 (98%)     | 0.04   | 1 (1%) 78 54   | 106, 130, 160, 174    | 0     |
| 45  | CL    | 120/267 (44%)   | 0.17   | 6 (5%) 34 19   | 100, 143, 178, 186    | 0     |
| 45  | i     | 106/267 (39%)   | 0.50   | 7 (6%) 24 15   | 108, 150, 178, 201    | 0     |
| 46  | B     | 1708/1787 (95%) | 0.33   | 100 (5%) 28 16 | 83, 128, 212, 439     | 0     |
| 46  | CM    | 1728/1787 (96%) | 0.16   | 55 (3%) 50 29  | 86, 131, 222, 410     | 0     |
| 47  | C     | 208/261 (79%)   | 0.33   | 10 (4%) 35 19  | 127, 161, 191, 201    | 0     |
| 47  | CN    | 208/261 (79%)   | 0.25   | 9 (4%) 40 21   | 101, 152, 181, 215    | 0     |
| 48  | CO    | 213/256 (83%)   | -0.08  | 5 (2%) 61 37   | 124, 173, 195, 212    | 0     |
| 48  | D     | 214/256 (83%)   | 0.15   | 5 (2%) 61 37   | 110, 144, 167, 178    | 0     |
| 49  | CP    | 217/249 (87%)   | 0.24   | 10 (4%) 37 20  | 83, 124, 152, 171     | 0     |
| 49  | E     | 217/249 (87%)   | 0.38   | 18 (8%) 17 11  | 106, 137, 164, 187    | 0     |
| 50  | CQ    | 223/251 (88%)   | 0.23   | 11 (4%) 35 19  | 99, 130, 186, 216     | 0     |
| 50  | F     | 223/251 (88%)   | 0.48   | 15 (6%) 24 15  | 103, 143, 197, 215    | 0     |
| 51  | CR    | 260/262 (99%)   | 0.20   | 17 (6%) 25 15  | 103, 130, 156, 184    | 0     |
| 51  | G     | 258/262 (98%)   | 0.78   | 27 (10%) 11 8  | 110, 145, 166, 192    | 0     |
| 52  | CS    | 205/225 (91%)   | 0.21   | 12 (5%) 28 16  | 124, 155, 189, 241    | 0     |
| 52  | H     | 206/225 (91%)   | 0.54   | 19 (9%) 14 9   | 107, 146, 181, 213    | 0     |
| 53  | CT    | 236/236 (100%)  | 0.32   | 9 (3%) 44 24   | 94, 143, 182, 203     | 0     |
| 53  | I     | 223/236 (94%)   | 0.47   | 24 (10%) 11 8  | 97, 143, 178, 222     | 0     |
| 54  | CU    | 179/186 (96%)   | -0.02  | 4 (2%) 62 37   | 123, 179, 214, 226    | 0     |
| 54  | J     | 182/186 (97%)   | 0.40   | 11 (6%) 27 16  | 118, 180, 204, 219    | 0     |
| 55  | CV    | 203/206 (98%)   | 0.57   | 21 (10%) 12 8  | 82, 121, 170, 195     | 0     |
| 55  | K     | 203/206 (98%)   | 0.34   | 16 (7%) 18 12  | 89, 129, 173, 189     | 0     |
| 56  | CW    | 178/189 (94%)   | 0.34   | 11 (6%) 26 16  | 101, 137, 167, 188    | 0     |
| 56  | L     | 178/189 (94%)   | 0.78   | 25 (14%) 6 5   | 118, 151, 173, 185    | 0     |
| 57  | CX    | 94/118 (79%)    | -0.04  | 0 100 100      | 104, 147, 177, 208    | 0     |
| 57  | M     | 98/118 (83%)    | 0.35   | 4 (4%) 41 22   | 108, 154, 188, 204    | 0     |
| 58  | CY    | 141/155 (90%)   | 0.16   | 1 (0%) 84 63   | 83, 118, 151, 197     | 0     |
| 58  | N     | 144/155 (92%)   | 0.50   | 12 (8%) 17 11  | 102, 129, 165, 189    | 0     |
| 59  | CZ    | 119/143 (83%)   | 0.03   | 1 (0%) 82 60   | 178, 214, 225, 231    | 0     |
| 59  | O     | 116/143 (81%)   | 0.21   | 5 (4%) 40 21   | 193, 225, 239, 248    | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------|-----|-----|-----------------------|-------|
| 60  | DA    | 150/151 (99%) | 0.29   | 6 (4%)   | 42  | 23  | 103, 146, 173, 183    | 0     |
| 60  | P     | 148/151 (98%) | 0.56   | 11 (7%)  | 20  | 13  | 101, 140, 167, 179    | 0     |
| 61  | DB    | 122/132 (92%) | 0.09   | 3 (2%)   | 58  | 35  | 98, 153, 179, 189     | 0     |
| 61  | Q     | 127/132 (96%) | 0.38   | 8 (6%)   | 26  | 15  | 97, 129, 152, 162     | 0     |
| 62  | DC    | 130/142 (91%) | 0.51   | 6 (4%)   | 37  | 20  | 115, 155, 184, 195    | 0     |
| 62  | R     | 131/142 (92%) | 0.41   | 8 (6%)   | 27  | 16  | 94, 138, 178, 202     | 0     |
| 63  | DD    | 139/142 (97%) | 0.69   | 16 (11%) | 9   | 6   | 108, 152, 179, 189    | 0     |
| 63  | S     | 139/142 (97%) | 0.59   | 13 (9%)  | 14  | 9   | 110, 149, 184, 201    | 0     |
| 64  | DE    | 124/137 (90%) | 0.43   | 6 (4%)   | 35  | 19  | 104, 163, 207, 216    | 0     |
| 64  | T     | 124/137 (90%) | 0.44   | 7 (5%)   | 30  | 17  | 128, 167, 217, 226    | 0     |
| 65  | DF    | 141/145 (97%) | 0.31   | 2 (1%)   | 73  | 48  | 115, 153, 182, 210    | 0     |
| 65  | U     | 144/145 (99%) | 0.28   | 4 (2%)   | 55  | 32  | 96, 126, 165, 179     | 0     |
| 66  | DG    | 141/145 (97%) | 0.30   | 4 (2%)   | 55  | 32  | 117, 150, 175, 193    | 0     |
| 66  | V     | 141/145 (97%) | 0.31   | 3 (2%)   | 63  | 38  | 110, 137, 176, 196    | 0     |
| 67  | DH    | 97/119 (81%)  | 0.58   | 9 (9%)   | 14  | 9   | 97, 147, 182, 194     | 0     |
| 67  | W     | 102/119 (85%) | 0.65   | 10 (9%)  | 13  | 9   | 96, 164, 192, 198     | 0     |
| 68  | DI    | 87/87 (100%)  | 0.15   | 3 (3%)   | 48  | 27  | 106, 144, 173, 193    | 0     |
| 68  | X     | 87/87 (100%)  | 0.14   | 2 (2%)   | 61  | 37  | 111, 147, 172, 181    | 0     |
| 69  | DJ    | 129/130 (99%) | 0.28   | 0        | 100 | 100 | 104, 127, 144, 151    | 0     |
| 69  | Y     | 129/130 (99%) | 0.58   | 5 (3%)   | 43  | 23  | 112, 133, 148, 154    | 0     |
| 70  | DK    | 143/145 (98%) | 0.52   | 10 (6%)  | 22  | 14  | 79, 104, 131, 156     | 0     |
| 70  | Z     | 143/145 (98%) | 0.58   | 12 (8%)  | 17  | 11  | 85, 110, 132, 158     | 0     |
| 71  | DL    | 132/135 (97%) | 0.02   | 2 (1%)   | 72  | 47  | 114, 150, 176, 204    | 0     |
| 71  | a     | 134/135 (99%) | 0.25   | 8 (5%)   | 27  | 16  | 115, 152, 175, 189    | 0     |
| 72  | DM    | 71/105 (67%)  | 0.04   | 1 (1%)   | 73  | 48  | 149, 175, 195, 201    | 0     |
| 72  | b     | 72/105 (68%)  | -0.06  | 1 (1%)   | 73  | 48  | 120, 150, 179, 193    | 0     |
| 73  | DN    | 98/119 (82%)  | 0.31   | 6 (6%)   | 27  | 16  | 109, 136, 188, 195    | 0     |
| 73  | c     | 97/119 (81%)  | 0.49   | 9 (9%)   | 14  | 9   | 100, 133, 168, 197    | 0     |
| 74  | DO    | 81/82 (98%)   | 0.02   | 1 (1%)   | 76  | 52  | 125, 163, 219, 233    | 0     |
| 74  | d     | 81/82 (98%)   | 0.35   | 4 (4%)   | 35  | 19  | 120, 154, 198, 218    | 0     |
| 75  | DP    | 61/67 (91%)   | -0.12  | 1 (1%)   | 70  | 45  | 133, 162, 183, 192    | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 75  | e     | 60/67 (89%)       | 0.32   | 5 (8%) 17 11    | 125, 156, 185, 191    | 0     |
| 76  | DQ    | 54/56 (96%)       | 0.50   | 3 (5%) 30 17    | 95, 116, 149, 169     | 0     |
| 76  | f     | 55/56 (98%)       | 0.89   | 8 (14%) 6 5     | 98, 118, 141, 175     | 0     |
| 77  | DR    | 59/63 (93%)       | 0.48   | 5 (8%) 16 11    | 98, 140, 207, 220     | 0     |
| 77  | g     | 60/63 (95%)       | 0.64   | 7 (11%) 9 6     | 117, 147, 202, 222    | 0     |
| 78  | DS    | 68/193 (35%)      | 0.20   | 4 (5%) 28 16    | 154, 226, 246, 252    | 0     |
| 78  | h     | 70/193 (36%)      | 0.47   | 7 (10%) 12 8    | 163, 211, 237, 252    | 0     |
| 79  | AR    | 311/317 (98%)     | 0.27   | 8 (2%) 57 33    | 162, 200, 225, 242    | 0     |
| 79  | DT    | 307/317 (96%)     | -0.01  | 4 (1%) 75 50    | 162, 200, 221, 236    | 0     |
| 80  | BE    | 205/220 (93%)     | 0.19   | 7 (3%) 48 27    | 64, 97, 143, 172      | 0     |
| 81  | P0    | 107/312 (34%)     | -0.05  | 1 (0%) 81 58    | 155, 176, 191, 202    | 0     |
| 82  | 12    | 63/165 (38%)      | -0.10  | 0 100 100       | 159, 180, 196, 207    | 0     |
| All | All   | 32813/35602 (92%) | 0.34   | 1793 (5%) 30 18 | 57, 128, 201, 439     | 0     |

All (1793) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 51  | G     | 39  | ARG  | 9.7  |
| 53  | I     | 79  | LYS  | 9.0  |
| 53  | CT    | 79  | LYS  | 8.9  |
| 6   | l     | 55  | GLU  | 8.6  |
| 35  | CB    | 33  | GLN  | 8.5  |
| 6   | AY    | 363 | ASN  | 8.2  |
| 63  | DD    | 129 | GLY  | 8.0  |
| 13  | BF    | 143 | ARG  | 8.0  |
| 16  | v     | 185 | ALA  | 8.0  |
| 60  | P     | 7   | SER  | 7.7  |
| 70  | Z     | 27  | GLN  | 7.6  |
| 8   | n     | 1   | MET  | 7.6  |
| 6   | AY    | 66  | TRP  | 7.6  |
| 63  | DD    | 137 | PHE  | 7.6  |
| 16  | v     | 184 | LYS  | 7.5  |
| 1   | AS    | 132 | U    | 7.5  |
| 29  | AB    | 46  | ASP  | 7.4  |
| 67  | DH    | 76  | LYS  | 7.3  |
| 16  | v     | 193 | LYS  | 7.2  |
| 32  | BY    | 26  | LYS  | 6.9  |
| 35  | CB    | 21  | LYS  | 6.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 51  | CR    | 2    | ALA  | 6.8  |
| 78  | DS    | 127  | TYR  | 6.8  |
| 7   | AZ    | 150  | LEU  | 6.8  |
| 46  | CM    | 1270 | U    | 6.7  |
| 76  | f     | 54   | LYS  | 6.7  |
| 35  | AH    | 61   | GLN  | 6.7  |
| 53  | I     | 86   | PRO  | 6.6  |
| 53  | I     | 80   | GLY  | 6.5  |
| 51  | G     | 6    | LYS  | 6.4  |
| 5   | AX    | 245  | GLY  | 6.4  |
| 40  | AM    | 34   | LYS  | 6.4  |
| 66  | DG    | 92   | LYS  | 6.3  |
| 6   | AY    | 70   | ARG  | 6.3  |
| 36  | CC    | 83   | LYS  | 6.3  |
| 35  | CB    | 20   | ILE  | 6.2  |
| 1   | 1     | 1127 | G    | 6.2  |
| 6   | AY    | 110  | TRP  | 6.2  |
| 70  | DK    | 27   | GLN  | 6.2  |
| 6   | AY    | 199  | ARG  | 6.2  |
| 7   | AZ    | 27   | LYS  | 6.2  |
| 16  | BI    | 89   | VAL  | 6.1  |
| 1   | AS    | 134  | U    | 6.0  |
| 46  | B     | 1016 | U    | 6.0  |
| 46  | B     | 1078 | A    | 5.9  |
| 33  | BZ    | 35   | LYS  | 5.9  |
| 29  | BV    | 110  | GLY  | 5.9  |
| 63  | DD    | 131  | ARG  | 5.9  |
| 19  | BL    | 168  | LYS  | 5.9  |
| 53  | I     | 77   | LEU  | 5.9  |
| 51  | G     | 14   | ALA  | 5.9  |
| 5   | k     | 23   | ALA  | 5.8  |
| 7   | AZ    | 149  | GLY  | 5.7  |
| 67  | DH    | 78   | TRP  | 5.7  |
| 22  | BO    | 79   | VAL  | 5.7  |
| 18  | x     | 128  | ARG  | 5.7  |
| 55  | CV    | 53   | GLN  | 5.7  |
| 1   | AS    | 368  | G    | 5.7  |
| 49  | CP    | 86   | ARG  | 5.6  |
| 9   | BB    | 126  | LYS  | 5.6  |
| 50  | F     | 188  | LYS  | 5.6  |
| 17  | w     | 30   | ASN  | 5.6  |
| 20  | BM    | 12   | ALA  | 5.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | CC           | 88         | LEU         | 5.5         |
| 55         | CV           | 40         | PRO         | 5.5         |
| 35         | CB           | 31         | VAL         | 5.5         |
| 35         | CB           | 35         | VAL         | 5.5         |
| 6          | AY           | 197        | GLY         | 5.5         |
| 46         | B            | 1099       | G           | 5.5         |
| 35         | CB           | 36         | LYS         | 5.5         |
| 16         | BI           | 189        | HIS         | 5.4         |
| 22         | BO           | 81         | GLY         | 5.4         |
| 6          | AY           | 361        | LEU         | 5.4         |
| 20         | z            | 54         | PRO         | 5.4         |
| 63         | DD           | 136        | ARG         | 5.4         |
| 46         | B            | 1571       | G           | 5.3         |
| 68         | DI           | 20         | THR         | 5.3         |
| 63         | S            | 129        | GLY         | 5.3         |
| 16         | BI           | 191        | TRP         | 5.3         |
| 63         | DD           | 128        | PHE         | 5.3         |
| 7          | AZ           | 53         | VAL         | 5.3         |
| 38         | AK           | 51         | LEU         | 5.3         |
| 33         | AF           | 53         | GLN         | 5.3         |
| 35         | CB           | 32         | ALA         | 5.3         |
| 19         | BL           | 160        | GLY         | 5.2         |
| 1          | AS           | 1927       | U           | 5.2         |
| 6          | AY           | 55         | GLU         | 5.2         |
| 46         | B            | 1399       | U           | 5.2         |
| 35         | CB           | 34         | HIS         | 5.2         |
| 53         | CT           | 158        | VAL         | 5.1         |
| 51         | G            | 2          | ALA         | 5.1         |
| 55         | CV           | 19         | ALA         | 5.1         |
| 47         | C            | 97         | ALA         | 5.1         |
| 70         | Z            | 31         | ALA         | 5.1         |
| 46         | B            | 1270       | U           | 5.1         |
| 8          | n            | 2          | SER         | 5.1         |
| 35         | AH           | 21         | LYS         | 5.1         |
| 1          | 1            | 1188       | C           | 5.1         |
| 1          | AS           | 1850       | C           | 5.1         |
| 6          | l            | 110        | TRP         | 5.0         |
| 20         | BM           | 93         | VAL         | 5.0         |
| 6          | AY           | 52         | ALA         | 5.0         |
| 6          | l            | 105        | LYS         | 5.0         |
| 46         | B            | 357        | A           | 5.0         |
| 20         | z            | 51         | VAL         | 5.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | l     | 199  | ARG  | 5.0  |
| 30  | BW    | 32   | LEU  | 5.0  |
| 35  | CB    | 61   | GLN  | 4.9  |
| 77  | g     | 35   | TYR  | 4.9  |
| 53  | I     | 97   | VAL  | 4.9  |
| 29  | BV    | 127  | ALA  | 4.9  |
| 60  | P     | 121  | ARG  | 4.9  |
| 16  | v     | 192  | LYS  | 4.8  |
| 1   | AS    | 826  | A    | 4.8  |
| 46  | CM    | 1571 | G    | 4.8  |
| 4   | AW    | 235  | ALA  | 4.8  |
| 47  | CN    | 74   | ALA  | 4.8  |
| 56  | L     | 51   | LYS  | 4.7  |
| 46  | B     | 75   | U    | 4.7  |
| 38  | CE    | 18   | LEU  | 4.7  |
| 1   | 1     | 949  | G    | 4.7  |
| 70  | Z     | 24   | TRP  | 4.7  |
| 24  | 6     | 137  | VAL  | 4.7  |
| 35  | AH    | 29   | LYS  | 4.6  |
| 53  | I     | 96   | SER  | 4.6  |
| 62  | R     | 17   | PHE  | 4.6  |
| 67  | DH    | 77   | THR  | 4.6  |
| 6   | l     | 59   | HIS  | 4.6  |
| 3   | AU    | 111  | A    | 4.6  |
| 53  | I     | 135  | PRO  | 4.6  |
| 67  | DH    | 63   | LYS  | 4.5  |
| 4   | j     | 195  | SER  | 4.5  |
| 46  | B     | 298  | A    | 4.5  |
| 16  | BI    | 81   | TYR  | 4.5  |
| 5   | AX    | 10   | ARG  | 4.5  |
| 4   | AW    | 228  | GLY  | 4.5  |
| 50  | F     | 167  | ASP  | 4.5  |
| 16  | v     | 174  | ILE  | 4.5  |
| 6   | AY    | 84   | HIS  | 4.5  |
| 1   | AS    | 1192 | C    | 4.5  |
| 46  | B     | 482  | C    | 4.5  |
| 47  | CN    | 134  | LYS  | 4.5  |
| 7   | m     | 92   | LEU  | 4.5  |
| 1   | AS    | 1862 | C    | 4.4  |
| 46  | CM    | 1099 | G    | 4.4  |
| 32  | BY    | 30   | LYS  | 4.4  |
| 33  | BZ    | 37   | LYS  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 77  | g     | 39   | LEU  | 4.4  |
| 35  | AH    | 38   | ALA  | 4.4  |
| 51  | G     | 13   | ALA  | 4.4  |
| 15  | BH    | 52   | LEU  | 4.4  |
| 52  | H     | 84   | LYS  | 4.4  |
| 18  | x     | 126  | ARG  | 4.4  |
| 29  | AB    | 17   | ALA  | 4.4  |
| 1   | AS    | 1483 | G    | 4.4  |
| 5   | AX    | 242  | THR  | 4.4  |
| 9   | BB    | 98   | ARG  | 4.3  |
| 1   | 1     | 1781 | C    | 4.3  |
| 1   | AS    | 1775 | C    | 4.3  |
| 1   | AS    | 2379 | A    | 4.3  |
| 46  | B     | 929  | A    | 4.3  |
| 51  | CR    | 39   | ARG  | 4.3  |
| 9   | o     | 90   | ILE  | 4.3  |
| 55  | K     | 53   | GLN  | 4.3  |
| 70  | Z     | 30   | LYS  | 4.3  |
| 46  | B     | 1404 | G    | 4.3  |
| 63  | DD    | 130  | GLY  | 4.3  |
| 35  | AH    | 22   | VAL  | 4.3  |
| 7   | AZ    | 61   | ILE  | 4.2  |
| 46  | B     | 938  | G    | 4.2  |
| 3   | AU    | 38   | U    | 4.2  |
| 46  | CM    | 1404 | G    | 4.2  |
| 51  | G     | 15   | PRO  | 4.2  |
| 16  | BI    | 146  | ALA  | 4.2  |
| 1   | 1     | 1197 | C    | 4.2  |
| 29  | AB    | 68   | PHE  | 4.2  |
| 45  | CL    | 103  | LEU  | 4.2  |
| 51  | G     | 45   | VAL  | 4.2  |
| 22  | BO    | 86   | GLU  | 4.2  |
| 49  | E     | 79   | ARG  | 4.2  |
| 51  | G     | 40   | GLU  | 4.2  |
| 9   | BB    | 96   | LYS  | 4.2  |
| 3   | AU    | 22   | U    | 4.2  |
| 1   | AS    | 1188 | C    | 4.2  |
| 67  | W     | 76   | LYS  | 4.2  |
| 1   | AS    | 2943 | A    | 4.2  |
| 45  | i     | 103  | LEU  | 4.2  |
| 80  | BE    | 199  | PHE  | 4.2  |
| 55  | K     | 45   | SER  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | y     | 69   | ARG  | 4.1  |
| 29  | BV    | 68   | PHE  | 4.1  |
| 70  | Z     | 21   | ASN  | 4.1  |
| 52  | H     | 76   | LYS  | 4.1  |
| 15  | u     | 128  | LEU  | 4.1  |
| 46  | CM    | 504  | A    | 4.1  |
| 46  | CM    | 1618 | A    | 4.1  |
| 79  | AR    | 134  | VAL  | 4.1  |
| 1   | AS    | 895  | U    | 4.1  |
| 63  | DD    | 126  | LYS  | 4.1  |
| 49  | E     | 80   | SER  | 4.1  |
| 46  | B     | 381  | G    | 4.1  |
| 6   | l     | 66   | TRP  | 4.0  |
| 56  | L     | 14   | VAL  | 4.0  |
| 46  | CM    | 1703 | C    | 4.0  |
| 52  | H     | 70   | VAL  | 4.0  |
| 78  | h     | 126  | VAL  | 4.0  |
| 27  | BT    | 16   | ARG  | 4.0  |
| 4   | j     | 110  | GLY  | 4.0  |
| 36  | CC    | 84   | LYS  | 4.0  |
| 51  | G     | 22   | LYS  | 4.0  |
| 6   | AY    | 106  | THR  | 4.0  |
| 56  | L     | 13   | SER  | 4.0  |
| 16  | BI    | 184  | LYS  | 4.0  |
| 70  | DK    | 21   | ASN  | 4.0  |
| 1   | 1     | 110  | C    | 4.0  |
| 1   | AS    | 1888 | G    | 4.0  |
| 46  | CM    | 382  | G    | 4.0  |
| 52  | CS    | 71   | SER  | 4.0  |
| 1   | 1     | 1934 | U    | 4.0  |
| 6   | l     | 104  | THR  | 4.0  |
| 17  | w     | 11   | ASP  | 4.0  |
| 36  | CC    | 92   | LEU  | 4.0  |
| 47  | C     | 130  | ALA  | 4.0  |
| 54  | J     | 89   | LEU  | 4.0  |
| 60  | P     | 5    | HIS  | 4.0  |
| 46  | B     | 1570 | A    | 3.9  |
| 52  | H     | 71   | SER  | 3.9  |
| 3   | 4     | 21   | C    | 3.9  |
| 6   | AY    | 188  | LEU  | 3.9  |
| 74  | d     | 24   | LEU  | 3.9  |
| 7   | AZ    | 62   | ALA  | 3.9  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | AS           | 827        | G           | 3.9         |
| 46         | B            | 1135       | G           | 3.9         |
| 7          | AZ           | 38         | THR         | 3.9         |
| 68         | X            | 58         | TYR         | 3.9         |
| 19         | y            | 180        | ARG         | 3.9         |
| 1          | 1            | 2454       | C           | 3.9         |
| 6          | l            | 195        | LEU         | 3.9         |
| 15         | u            | 13         | VAL         | 3.9         |
| 16         | BI           | 174        | ILE         | 3.9         |
| 46         | B            | 259        | U           | 3.9         |
| 10         | BC           | 67         | SER         | 3.9         |
| 1          | AS           | 775        | G           | 3.9         |
| 7          | AZ           | 54         | ARG         | 3.9         |
| 53         | CT           | 135        | PRO         | 3.9         |
| 51         | G            | 47         | PHE         | 3.9         |
| 19         | BL           | 159        | LYS         | 3.9         |
| 41         | CH           | 23         | CYS         | 3.8         |
| 46         | B            | 1359       | U           | 3.8         |
| 4          | j            | 153        | GLY         | 3.8         |
| 63         | DD           | 135        | ALA         | 3.8         |
| 78         | DS           | 126        | VAL         | 3.8         |
| 2          | AT           | 73         | C           | 3.8         |
| 1          | 1            | 2090       | U           | 3.8         |
| 33         | AF           | 35         | LYS         | 3.8         |
| 79         | AR           | 138        | ILE         | 3.8         |
| 41         | CH           | 37         | ARG         | 3.8         |
| 49         | E            | 203        | GLU         | 3.8         |
| 16         | v            | 153        | ASN         | 3.8         |
| 1          | AS           | 1891       | A           | 3.8         |
| 75         | e            | 49         | ARG         | 3.8         |
| 1          | AS           | 1117       | U           | 3.8         |
| 46         | B            | 258        | U           | 3.8         |
| 22         | 2            | 77         | ASN         | 3.8         |
| 56         | CW           | 104        | PHE         | 3.8         |
| 76         | f            | 43         | PHE         | 3.8         |
| 35         | CB           | 22         | VAL         | 3.8         |
| 1          | 1            | 29         | G           | 3.8         |
| 54         | J            | 132        | ILE         | 3.8         |
| 52         | CS           | 113        | ILE         | 3.7         |
| 6          | l            | 91         | PHE         | 3.7         |
| 49         | CP           | 210        | PHE         | 3.7         |
| 11         | BD           | 9          | ILE         | 3.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | BL    | 84   | VAL  | 3.7  |
| 67  | DH    | 81   | TYR  | 3.7  |
| 55  | CV    | 45   | SER  | 3.7  |
| 6   | AY    | 362  | LYS  | 3.7  |
| 60  | P     | 9    | LYS  | 3.7  |
| 51  | CR    | 31   | PRO  | 3.7  |
| 20  | BM    | 19   | LYS  | 3.7  |
| 36  | AI    | 84   | LYS  | 3.7  |
| 1   | AS    | 774  | U    | 3.7  |
| 5   | AX    | 246  | LEU  | 3.7  |
| 49  | E     | 178  | VAL  | 3.7  |
| 53  | I     | 73   | VAL  | 3.7  |
| 73  | c     | 29   | CYS  | 3.7  |
| 63  | S     | 137  | PHE  | 3.7  |
| 16  | BI    | 193  | LYS  | 3.7  |
| 22  | 2     | 81   | GLY  | 3.7  |
| 51  | G     | 38   | LEU  | 3.7  |
| 52  | H     | 177  | ILE  | 3.7  |
| 63  | S     | 68   | VAL  | 3.7  |
| 22  | 2     | 84   | TYR  | 3.7  |
| 29  | AB    | 129  | PHE  | 3.7  |
| 19  | BL    | 5    | HIS  | 3.7  |
| 22  | BO    | 63   | ILE  | 3.7  |
| 50  | CQ    | 185  | ILE  | 3.7  |
| 11  | BD    | 10   | LEU  | 3.7  |
| 32  | AE    | 15   | LEU  | 3.7  |
| 46  | B     | 1392 | A    | 3.6  |
| 25  | BR    | 86   | SER  | 3.6  |
| 1   | 1     | 1192 | C    | 3.6  |
| 5   | AX    | 12   | GLY  | 3.6  |
| 38  | CE    | 23   | GLY  | 3.6  |
| 7   | m     | 55   | PHE  | 3.6  |
| 6   | AY    | 234  | LEU  | 3.6  |
| 80  | BE    | 175  | PRO  | 3.6  |
| 5   | AX    | 4    | ARG  | 3.6  |
| 6   | AY    | 77   | ARG  | 3.6  |
| 36  | CC    | 91   | LYS  | 3.6  |
| 38  | CE    | 48   | ASN  | 3.6  |
| 63  | DD    | 127  | LYS  | 3.6  |
| 5   | k     | 217  | VAL  | 3.6  |
| 33  | AF    | 43   | VAL  | 3.6  |
| 47  | CN    | 107  | PHE  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 51  | CR    | 23   | LEU  | 3.6  |
| 67  | W     | 81   | TYR  | 3.6  |
| 77  | DR    | 35   | TYR  | 3.6  |
| 49  | CP    | 156  | LYS  | 3.6  |
| 56  | CW    | 10   | LYS  | 3.6  |
| 1   | AS    | 1217 | A    | 3.6  |
| 6   | l     | 61   | THR  | 3.6  |
| 24  | 6     | 22   | VAL  | 3.6  |
| 24  | BQ    | 49   | LEU  | 3.6  |
| 33  | BZ    | 36   | GLN  | 3.6  |
| 52  | H     | 87   | CYS  | 3.6  |
| 16  | v     | 173  | GLY  | 3.6  |
| 49  | E     | 214  | GLY  | 3.6  |
| 26  | BS    | 60   | HIS  | 3.6  |
| 42  | CI    | 10   | VAL  | 3.6  |
| 50  | F     | 207  | VAL  | 3.6  |
| 67  | W     | 79   | ASP  | 3.6  |
| 1   | 1     | 1138 | G    | 3.6  |
| 52  | CS    | 177  | ILE  | 3.6  |
| 1   | AS    | 2382 | A    | 3.6  |
| 8   | BA    | 69   | LYS  | 3.6  |
| 29  | BV    | 72   | GLU  | 3.6  |
| 61  | DB    | 85   | LYS  | 3.6  |
| 6   | l     | 90   | ALA  | 3.6  |
| 63  | DD    | 134  | ARG  | 3.6  |
| 70  | Z     | 28   | ALA  | 3.6  |
| 13  | s     | 19   | LEU  | 3.6  |
| 29  | AB    | 45   | LEU  | 3.6  |
| 64  | T     | 9    | VAL  | 3.6  |
| 7   | AZ    | 69   | ILE  | 3.5  |
| 22  | BO    | 32   | LYS  | 3.5  |
| 22  | 2     | 86   | GLU  | 3.5  |
| 18  | x     | 22   | LEU  | 3.5  |
| 76  | f     | 40   | ARG  | 3.5  |
| 9   | o     | 132  | VAL  | 3.5  |
| 18  | BK    | 77   | GLY  | 3.5  |
| 6   | AY    | 353  | SER  | 3.5  |
| 5   | AX    | 236  | LYS  | 3.5  |
| 33  | AF    | 37   | LYS  | 3.5  |
| 45  | CL    | 98   | ASP  | 3.5  |
| 10  | BC    | 151  | LEU  | 3.5  |
| 27  | BT    | 76   | LEU  | 3.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 56         | CW           | 15         | PRO         | 3.5         |
| 56         | L            | 47         | PHE         | 3.5         |
| 1          | AS           | 780        | A           | 3.5         |
| 1          | AS           | 2098       | A           | 3.5         |
| 1          | AS           | 3320       | U           | 3.5         |
| 5          | AX           | 249        | VAL         | 3.5         |
| 55         | CV           | 51         | GLY         | 3.5         |
| 58         | N            | 70         | ILE         | 3.5         |
| 7          | m            | 82         | GLU         | 3.5         |
| 35         | AH           | 32         | ALA         | 3.5         |
| 49         | E            | 161        | ALA         | 3.5         |
| 52         | H            | 61         | TYR         | 3.5         |
| 4          | j            | 13         | GLY         | 3.5         |
| 8          | BA           | 66         | GLY         | 3.5         |
| 11         | BD           | 8          | GLN         | 3.5         |
| 55         | CV           | 20         | GLN         | 3.5         |
| 1          | AS           | 1906       | A           | 3.5         |
| 22         | BO           | 77         | ASN         | 3.5         |
| 46         | B            | 504        | A           | 3.5         |
| 6          | AY           | 224        | PRO         | 3.5         |
| 26         | 8            | 66         | PRO         | 3.5         |
| 14         | t            | 20         | GLU         | 3.5         |
| 49         | E            | 77         | LYS         | 3.5         |
| 34         | AG           | 95         | GLY         | 3.5         |
| 7          | m            | 24         | GLN         | 3.5         |
| 51         | CR           | 6          | LYS         | 3.4         |
| 46         | B            | 1615       | U           | 3.4         |
| 46         | CM           | 1292       | U           | 3.4         |
| 17         | BJ           | 53         | LEU         | 3.4         |
| 19         | BL           | 156        | GLY         | 3.4         |
| 45         | CL           | 84         | SER         | 3.4         |
| 79         | AR           | 82         | LEU         | 3.4         |
| 29         | AB           | 65         | GLN         | 3.4         |
| 45         | i            | 42         | ALA         | 3.4         |
| 46         | B            | 1390       | C           | 3.4         |
| 33         | AF           | 36         | GLN         | 3.4         |
| 16         | BI           | 74         | PRO         | 3.4         |
| 20         | z            | 52         | LYS         | 3.4         |
| 46         | B            | 393        | U           | 3.4         |
| 1          | AS           | 402        | A           | 3.4         |
| 1          | AS           | 2364       | A           | 3.4         |
| 5          | k            | 107        | ALA         | 3.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | CN    | 130  | ALA  | 3.4  |
| 20  | z     | 17   | VAL  | 3.4  |
| 16  | v     | 108  | ARG  | 3.4  |
| 1   | AS    | 171  | G    | 3.4  |
| 1   | AS    | 1138 | G    | 3.4  |
| 35  | AH    | 36   | LYS  | 3.4  |
| 16  | BI    | 175  | ASN  | 3.4  |
| 5   | AX    | 250  | ALA  | 3.4  |
| 10  | BC    | 200  | ALA  | 3.4  |
| 55  | CV    | 79   | ALA  | 3.4  |
| 50  | F     | 40   | VAL  | 3.4  |
| 1   | 1     | 780  | A    | 3.4  |
| 1   | 1     | 2466 | A    | 3.4  |
| 30  | BW    | 5    | LYS  | 3.4  |
| 56  | L     | 2    | PRO  | 3.4  |
| 16  | BI    | 43   | SER  | 3.4  |
| 4   | AW    | 3    | ARG  | 3.4  |
| 49  | E     | 210  | PHE  | 3.4  |
| 56  | L     | 104  | PHE  | 3.4  |
| 1   | 1     | 102  | G    | 3.4  |
| 5   | k     | 24   | LYS  | 3.4  |
| 24  | BQ    | 15   | LEU  | 3.4  |
| 52  | H     | 86   | GLN  | 3.4  |
| 1   | 1     | 78   | U    | 3.4  |
| 1   | 1     | 2701 | U    | 3.4  |
| 6   | AY    | 122  | ALA  | 3.4  |
| 52  | CS    | 70   | VAL  | 3.4  |
| 16  | BI    | 108  | ARG  | 3.4  |
| 19  | BL    | 178  | ARG  | 3.4  |
| 33  | BZ    | 21   | HIS  | 3.4  |
| 67  | DH    | 67   | ARG  | 3.4  |
| 11  | q     | 71   | VAL  | 3.3  |
| 33  | BZ    | 45   | ARG  | 3.3  |
| 4   | AW    | 2    | GLY  | 3.3  |
| 17  | BJ    | 44   | ILE  | 3.3  |
| 26  | 8     | 123  | TYR  | 3.3  |
| 38  | CE    | 2    | GLY  | 3.3  |
| 9   | BB    | 103  | LEU  | 3.3  |
| 13  | s     | 147  | THR  | 3.3  |
| 52  | H     | 181  | GLU  | 3.3  |
| 1   | AS    | 133  | U    | 3.3  |
| 77  | DR    | 34   | ALA  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | I     | 74   | ARG  | 3.3  |
| 55  | CV    | 8    | ARG  | 3.3  |
| 9   | BB    | 101  | LEU  | 3.3  |
| 51  | G     | 52   | LEU  | 3.3  |
| 78  | DS    | 133  | ILE  | 3.3  |
| 51  | G     | 82   | TYR  | 3.3  |
| 6   | l     | 107  | TRP  | 3.3  |
| 9   | o     | 96   | LYS  | 3.3  |
| 1   | 1     | 659  | G    | 3.3  |
| 1   | 1     | 1405 | G    | 3.3  |
| 1   | 1     | 2700 | G    | 3.3  |
| 24  | 6     | 87   | ARG  | 3.3  |
| 46  | B     | 502  | U    | 3.3  |
| 6   | l     | 56   | ASN  | 3.3  |
| 20  | z     | 128  | LYS  | 3.3  |
| 13  | BF    | 76   | ALA  | 3.3  |
| 40  | AM    | 32   | ASP  | 3.3  |
| 54  | J     | 55   | ALA  | 3.3  |
| 9   | o     | 84   | VAL  | 3.3  |
| 46  | B     | 9    | U    | 3.3  |
| 46  | CM    | 1459 | U    | 3.3  |
| 47  | C     | 134  | LYS  | 3.3  |
| 73  | c     | 19   | LYS  | 3.3  |
| 1   | AS    | 174  | C    | 3.3  |
| 1   | AS    | 1419 | C    | 3.3  |
| 1   | 1     | 108  | A    | 3.3  |
| 1   | AS    | 1585 | A    | 3.3  |
| 5   | k     | 331  | VAL  | 3.3  |
| 12  | r     | 166  | ILE  | 3.3  |
| 35  | CB    | 8    | ARG  | 3.3  |
| 38  | CE    | 29   | VAL  | 3.3  |
| 54  | J     | 69   | VAL  | 3.3  |
| 20  | BM    | 16   | GLY  | 3.3  |
| 17  | BJ    | 129  | ARG  | 3.2  |
| 1   | 1     | 1933 | U    | 3.2  |
| 46  | B     | 797  | U    | 3.2  |
| 1   | AS    | 1197 | C    | 3.2  |
| 2   | 3     | 10   | C    | 3.2  |
| 4   | AW    | 236  | GLY  | 3.2  |
| 16  | v     | 196  | THR  | 3.2  |
| 16  | v     | 73   | ARG  | 3.2  |
| 30  | BW    | 14   | ARG  | 3.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 52         | H            | 152        | SER         | 3.2         |
| 5          | AX           | 263        | THR         | 3.2         |
| 7          | m            | 150        | LEU         | 3.2         |
| 14         | t            | 4          | SER         | 3.2         |
| 43         | CJ           | 84         | PRO         | 3.2         |
| 19         | y            | 185        | LYS         | 3.2         |
| 46         | B            | 740        | A           | 3.2         |
| 46         | B            | 1061       | A           | 3.2         |
| 52         | CS           | 115        | LYS         | 3.2         |
| 33         | AF           | 32         | ASN         | 3.2         |
| 51         | CR           | 4          | GLY         | 3.2         |
| 78         | DS           | 128        | THR         | 3.2         |
| 15         | u            | 122        | PHE         | 3.2         |
| 15         | BH           | 50         | ILE         | 3.2         |
| 70         | Z            | 17         | VAL         | 3.2         |
| 4          | AW           | 155        | LYS         | 3.2         |
| 7          | AZ           | 84         | PRO         | 3.2         |
| 1          | AS           | 1374       | U           | 3.2         |
| 1          | AS           | 1890       | U           | 3.2         |
| 34         | AG           | 14         | ILE         | 3.2         |
| 40         | CG           | 32         | ASP         | 3.2         |
| 70         | Z            | 32         | ARG         | 3.2         |
| 1          | AS           | 3054       | C           | 3.2         |
| 46         | B            | 1066       | A           | 3.2         |
| 46         | CM           | 674        | C           | 3.2         |
| 44         | AQ           | 6          | LYS         | 3.2         |
| 46         | B            | 1068       | G           | 3.2         |
| 76         | f            | 52         | PHE         | 3.2         |
| 4          | AW           | 6          | ARG         | 3.2         |
| 58         | N            | 97         | TYR         | 3.2         |
| 29         | BV           | 126        | LYS         | 3.2         |
| 10         | BC           | 199        | ALA         | 3.2         |
| 53         | I            | 75         | LEU         | 3.2         |
| 6          | AY           | 200        | PHE         | 3.1         |
| 11         | BD           | 53         | ILE         | 3.1         |
| 1          | 1            | 703        | A           | 3.1         |
| 1          | 1            | 2467       | C           | 3.1         |
| 35         | AH           | 14         | ASN         | 3.1         |
| 19         | y            | 159        | LYS         | 3.1         |
| 30         | BW           | 33         | LYS         | 3.1         |
| 45         | CL           | 100        | LYS         | 3.1         |
| 27         | BT           | 73         | VAL         | 3.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | CC           | 82         | ALA         | 3.1         |
| 37         | CD           | 8          | ALA         | 3.1         |
| 16         | BI           | 197        | LEU         | 3.1         |
| 1          | AS           | 883        | G           | 3.1         |
| 46         | CM           | 1672       | G           | 3.1         |
| 1          | AS           | 1661       | U           | 3.1         |
| 3          | AU           | 23         | U           | 3.1         |
| 46         | CM           | 1590       | U           | 3.1         |
| 19         | BL           | 161        | LYS         | 3.1         |
| 16         | BI           | 195        | ASN         | 3.1         |
| 68         | DI           | 58         | TYR         | 3.1         |
| 53         | CT           | 153        | VAL         | 3.1         |
| 63         | DD           | 133        | ALA         | 3.1         |
| 46         | CM           | 1322       | A           | 3.1         |
| 3          | 4            | 91         | C           | 3.1         |
| 56         | CW           | 2          | PRO         | 3.1         |
| 16         | BI           | 144        | ARG         | 3.1         |
| 35         | AH           | 8          | ARG         | 3.1         |
| 38         | CE           | 10         | LYS         | 3.1         |
| 79         | DT           | 106        | GLY         | 3.1         |
| 56         | L            | 48         | GLN         | 3.1         |
| 49         | E            | 81         | VAL         | 3.1         |
| 9          | BB           | 123        | GLU         | 3.1         |
| 1          | 1            | 1602       | U           | 3.1         |
| 28         | AA           | 25         | ILE         | 3.1         |
| 46         | B            | 1614       | U           | 3.1         |
| 46         | CM           | 1614       | U           | 3.1         |
| 26         | 8            | 49         | LYS         | 3.1         |
| 16         | v            | 189        | HIS         | 3.1         |
| 29         | AB           | 11         | HIS         | 3.1         |
| 1          | 1            | 369        | A           | 3.1         |
| 1          | 1            | 947        | A           | 3.1         |
| 20         | z            | 7          | GLN         | 3.1         |
| 79         | AR           | 137        | THR         | 3.1         |
| 46         | B            | 1410       | A           | 3.1         |
| 8          | BA           | 51         | VAL         | 3.1         |
| 14         | BG           | 124        | VAL         | 3.1         |
| 20         | BM           | 13         | SER         | 3.1         |
| 29         | AB           | 66         | ASN         | 3.1         |
| 37         | CD           | 10         | VAL         | 3.1         |
| 46         | CM           | 1514       | C           | 3.1         |
| 58         | N            | 94         | VAL         | 3.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 60  | DA    | 84   | ILE  | 3.1  |
| 5   | AX    | 19   | ARG  | 3.1  |
| 16  | BI    | 77   | LYS  | 3.1  |
| 16  | BI    | 176  | LYS  | 3.1  |
| 50  | CQ    | 186  | LYS  | 3.1  |
| 55  | K     | 22   | ARG  | 3.1  |
| 55  | CV    | 22   | ARG  | 3.1  |
| 72  | b     | 34   | ASP  | 3.1  |
| 77  | DR    | 39   | LEU  | 3.1  |
| 1   | 1     | 329  | U    | 3.1  |
| 1   | AS    | 825  | U    | 3.1  |
| 3   | 4     | 23   | U    | 3.1  |
| 4   | AW    | 47   | GLN  | 3.1  |
| 35  | AH    | 23   | VAL  | 3.1  |
| 60  | DA    | 65   | VAL  | 3.1  |
| 5   | AX    | 6    | TYR  | 3.1  |
| 7   | AZ    | 49   | TYR  | 3.1  |
| 67  | W     | 78   | TRP  | 3.1  |
| 7   | m     | 25   | GLU  | 3.1  |
| 78  | h     | 130  | PRO  | 3.1  |
| 1   | 1     | 402  | A    | 3.1  |
| 1   | AS    | 917  | A    | 3.1  |
| 35  | AH    | 30   | LEU  | 3.1  |
| 44  | AQ    | 29   | LEU  | 3.1  |
| 54  | J     | 122  | LEU  | 3.1  |
| 46  | B     | 1067 | C    | 3.1  |
| 46  | CM    | 1144 | C    | 3.1  |
| 4   | AW    | 250  | GLN  | 3.0  |
| 33  | BZ    | 53   | GLN  | 3.0  |
| 8   | BA    | 143  | ALA  | 3.0  |
| 44  | AQ    | 61   | LYS  | 3.0  |
| 47  | C     | 102  | PHE  | 3.0  |
| 70  | DK    | 24   | TRP  | 3.0  |
| 46  | B     | 1376 | U    | 3.0  |
| 1   | AS    | 29   | G    | 3.0  |
| 16  | v     | 183  | THR  | 3.0  |
| 56  | L     | 45   | ILE  | 3.0  |
| 73  | c     | 18   | VAL  | 3.0  |
| 1   | AS    | 2323 | A    | 3.0  |
| 9   | o     | 126  | LYS  | 3.0  |
| 6   | l     | 48   | ARG  | 3.0  |
| 13  | s     | 145  | ARG  | 3.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 55         | K            | 8          | ARG         | 3.0         |
| 6          | AY           | 359        | GLU         | 3.0         |
| 56         | L            | 116        | LEU         | 3.0         |
| 1          | AS           | 2383       | C           | 3.0         |
| 46         | CM           | 1704       | C           | 3.0         |
| 56         | L            | 101        | PRO         | 3.0         |
| 6          | AY           | 87         | GLY         | 3.0         |
| 1          | 1            | 875        | U           | 3.0         |
| 1          | 1            | 962        | U           | 3.0         |
| 35         | AH           | 35         | VAL         | 3.0         |
| 46         | B            | 1292       | U           | 3.0         |
| 49         | E            | 196        | SER         | 3.0         |
| 49         | E            | 207        | LYS         | 3.0         |
| 63         | S            | 67         | LYS         | 3.0         |
| 14         | BG           | 2          | ALA         | 3.0         |
| 55         | CV           | 185        | CYS         | 3.0         |
| 56         | L            | 118        | LEU         | 3.0         |
| 4          | AW           | 73         | GLU         | 3.0         |
| 73         | c            | 20         | PRO         | 3.0         |
| 73         | c            | 31         | PRO         | 3.0         |
| 1          | 1            | 79         | G           | 3.0         |
| 1          | AS           | 863        | G           | 3.0         |
| 46         | B            | 382        | G           | 3.0         |
| 1          | AS           | 824        | A           | 3.0         |
| 20         | z            | 16         | GLY         | 3.0         |
| 46         | B            | 621        | A           | 3.0         |
| 46         | CM           | 1570       | A           | 3.0         |
| 35         | AH           | 37         | LYS         | 3.0         |
| 67         | W            | 63         | LYS         | 3.0         |
| 42         | CI           | 3          | ASP         | 3.0         |
| 67         | DH           | 93         | GLN         | 3.0         |
| 74         | DO           | 27         | GLN         | 3.0         |
| 22         | 2            | 79         | VAL         | 3.0         |
| 50         | F            | 150        | SER         | 3.0         |
| 26         | 8            | 82         | LEU         | 3.0         |
| 46         | B            | 1081       | C           | 3.0         |
| 69         | Y            | 41         | MET         | 3.0         |
| 22         | BO           | 84         | TYR         | 3.0         |
| 53         | I            | 83         | CYS         | 3.0         |
| 66         | V            | 18         | TYR         | 3.0         |
| 1          | AS           | 1778       | U           | 3.0         |
| 46         | B            | 1114       | U           | 3.0         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 18         | x            | 136        | ILE         | 3.0         |
| 30         | AC           | 22         | LYS         | 3.0         |
| 49         | E            | 78         | ILE         | 3.0         |
| 6          | AY           | 67         | GLY         | 3.0         |
| 35         | CB           | 3          | GLN         | 3.0         |
| 9          | BB           | 16         | ALA         | 3.0         |
| 51         | G            | 3          | ARG         | 3.0         |
| 1          | AS           | 1889       | A           | 3.0         |
| 4          | AW           | 219        | ILE         | 3.0         |
| 12         | r            | 167        | ILE         | 3.0         |
| 1          | 1            | 1406       | C           | 3.0         |
| 7          | AZ           | 170        | GLY         | 3.0         |
| 46         | CM           | 656        | C           | 3.0         |
| 77         | g            | 38         | LEU         | 3.0         |
| 1          | 1            | 3240       | U           | 3.0         |
| 5          | AX           | 8          | ALA         | 3.0         |
| 42         | AO           | 3          | ASP         | 3.0         |
| 7          | m            | 64         | ILE         | 2.9         |
| 41         | CH           | 3          | GLU         | 2.9         |
| 73         | c            | 3          | LYS         | 2.9         |
| 78         | h            | 123        | LYS         | 2.9         |
| 53         | I            | 156        | PHE         | 2.9         |
| 35         | CB           | 28         | GLY         | 2.9         |
| 55         | K            | 183        | GLY         | 2.9         |
| 8          | BA           | 157        | GLN         | 2.9         |
| 17         | BJ           | 45         | SER         | 2.9         |
| 1          | 1            | 408        | A           | 2.9         |
| 5          | AX           | 240        | ARG         | 2.9         |
| 6          | AY           | 72         | VAL         | 2.9         |
| 49         | E            | 202        | THR         | 2.9         |
| 55         | CV           | 46         | VAL         | 2.9         |
| 46         | CM           | 1184       | G           | 2.9         |
| 5          | AX           | 237        | LYS         | 2.9         |
| 1          | 1            | 3054       | C           | 2.9         |
| 29         | BV           | 11         | HIS         | 2.9         |
| 46         | CM           | 726        | C           | 2.9         |
| 56         | L            | 12         | TYR         | 2.9         |
| 7          | AZ           | 25         | GLU         | 2.9         |
| 56         | L            | 114        | PHE         | 2.9         |
| 9          | o            | 223        | GLY         | 2.9         |
| 18         | x            | 135        | ARG         | 2.9         |
| 17         | BJ           | 93         | THR         | 2.9         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | 8     | 51   | VAL  | 2.9  |
| 33  | BZ    | 43   | VAL  | 2.9  |
| 62  | R     | 76   | VAL  | 2.9  |
| 36  | AI    | 91   | LYS  | 2.9  |
| 49  | CP    | 78   | ILE  | 2.9  |
| 51  | G     | 9    | LEU  | 2.9  |
| 6   | l     | 200  | PHE  | 2.9  |
| 53  | CT    | 91   | GLU  | 2.9  |
| 53  | I     | 88   | ARG  | 2.9  |
| 64  | T     | 5    | ARG  | 2.9  |
| 35  | AH    | 33   | GLN  | 2.9  |
| 61  | Q     | 116  | VAL  | 2.9  |
| 1   | 1     | 1114 | C    | 2.9  |
| 1   | 1     | 1352 | C    | 2.9  |
| 1   | AS    | 30   | C    | 2.9  |
| 46  | CM    | 1182 | C    | 2.9  |
| 70  | DK    | 39   | LYS  | 2.9  |
| 1   | AS    | 1817 | U    | 2.9  |
| 1   | AS    | 1851 | U    | 2.9  |
| 2   | 3     | 16   | U    | 2.9  |
| 35  | CB    | 30   | LEU  | 2.9  |
| 29  | BV    | 46   | ASP  | 2.9  |
| 52  | H     | 100  | ASN  | 2.9  |
| 13  | s     | 130  | VAL  | 2.9  |
| 64  | T     | 4    | VAL  | 2.9  |
| 19  | y     | 168  | LYS  | 2.9  |
| 38  | AK    | 54   | LYS  | 2.9  |
| 50  | F     | 206  | ALA  | 2.9  |
| 33  | AF    | 51   | ILE  | 2.9  |
| 1   | 1     | 717  | A    | 2.9  |
| 1   | AS    | 1116 | A    | 2.9  |
| 46  | CM    | 383  | A    | 2.9  |
| 4   | j     | 246  | LEU  | 2.9  |
| 54  | CU    | 63   | LEU  | 2.9  |
| 77  | DR    | 30   | PRO  | 2.9  |
| 1   | 1     | 545  | G    | 2.9  |
| 46  | B     | 480  | U    | 2.9  |
| 46  | B     | 494  | G    | 2.9  |
| 53  | I     | 78   | SER  | 2.9  |
| 56  | L     | 130  | THR  | 2.9  |
| 14  | BG    | 89   | TYR  | 2.9  |
| 41  | CH    | 29   | PRO  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | CN    | 127  | ARG  | 2.9  |
| 55  | K     | 75   | LYS  | 2.9  |
| 28  | BU    | 26   | VAL  | 2.8  |
| 46  | CM    | 105  | A    | 2.8  |
| 22  | BO    | 149  | GLN  | 2.8  |
| 39  | CF    | 76   | THR  | 2.8  |
| 62  | DC    | 84   | ILE  | 2.8  |
| 14  | t     | 2    | ALA  | 2.8  |
| 19  | y     | 71   | LEU  | 2.8  |
| 51  | CR    | 9    | LEU  | 2.8  |
| 13  | s     | 102  | PHE  | 2.8  |
| 71  | a     | 23   | PHE  | 2.8  |
| 46  | B     | 615  | U    | 2.8  |
| 46  | CM    | 1400 | U    | 2.8  |
| 77  | g     | 36   | MET  | 2.8  |
| 22  | BO    | 5    | ARG  | 2.8  |
| 1   | 1     | 63   | G    | 2.8  |
| 1   | AS    | 980  | G    | 2.8  |
| 1   | AS    | 1664 | G    | 2.8  |
| 15  | u     | 117  | LYS  | 2.8  |
| 46  | B     | 1402 | G    | 2.8  |
| 41  | AN    | 23   | CYS  | 2.8  |
| 4   | AW    | 4    | VAL  | 2.8  |
| 4   | j     | 250  | GLN  | 2.8  |
| 7   | m     | 163  | LEU  | 2.8  |
| 7   | AZ    | 39   | GLN  | 2.8  |
| 11  | BD    | 158  | ALA  | 2.8  |
| 77  | g     | 37   | ARG  | 2.8  |
| 30  | AC    | 21   | ILE  | 2.8  |
| 47  | CN    | 121  | VAL  | 2.8  |
| 45  | i     | 137  | ASP  | 2.8  |
| 48  | D     | 156  | ALA  | 2.8  |
| 46  | B     | 392  | C    | 2.8  |
| 16  | v     | 191  | TRP  | 2.8  |
| 6   | AY    | 47   | LYS  | 2.8  |
| 16  | BI    | 72   | LYS  | 2.8  |
| 7   | AZ    | 146  | LEU  | 2.8  |
| 50  | F     | 159  | ILE  | 2.8  |
| 79  | AR    | 123  | ILE  | 2.8  |
| 24  | 6     | 55   | GLY  | 2.8  |
| 1   | 1     | 1499 | A    | 2.8  |
| 16  | BI    | 185  | ALA  | 2.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 46         | CM           | 1357       | A           | 2.8         |
| 6          | AY           | 186        | LYS         | 2.8         |
| 7          | AZ           | 50         | ARG         | 2.8         |
| 51         | CR           | 3          | ARG         | 2.8         |
| 1          | AS           | 1849       | U           | 2.8         |
| 46         | B            | 318        | U           | 2.8         |
| 46         | B            | 1401       | U           | 2.8         |
| 4          | j            | 210        | PRO         | 2.8         |
| 6          | AY           | 223        | VAL         | 2.8         |
| 35         | AH           | 31         | VAL         | 2.8         |
| 10         | BC           | 62         | GLN         | 2.8         |
| 43         | CJ           | 47         | GLN         | 2.8         |
| 43         | CJ           | 56         | GLN         | 2.8         |
| 8          | BA           | 80         | ALA         | 2.8         |
| 21         | 0            | 116        | ALA         | 2.8         |
| 22         | 2            | 24         | ALA         | 2.8         |
| 44         | AQ           | 28         | LYS         | 2.8         |
| 60         | P            | 109        | LYS         | 2.8         |
| 74         | d            | 22         | LYS         | 2.8         |
| 46         | B            | 939        | G           | 2.8         |
| 67         | DH           | 79         | ASP         | 2.8         |
| 73         | c            | 89         | ARG         | 2.8         |
| 4          | AW           | 225        | ILE         | 2.8         |
| 1          | 1            | 963        | A           | 2.8         |
| 1          | 1            | 2091       | A           | 2.8         |
| 1          | AS           | 1139       | A           | 2.8         |
| 19         | BL           | 83         | VAL         | 2.8         |
| 22         | BO           | 72         | VAL         | 2.8         |
| 70         | DK           | 17         | VAL         | 2.8         |
| 9          | o            | 222        | GLN         | 2.8         |
| 16         | v            | 104        | GLU         | 2.8         |
| 16         | BI           | 11         | GLN         | 2.8         |
| 29         | AB           | 72         | GLU         | 2.8         |
| 5          | AX           | 28         | ARG         | 2.7         |
| 63         | S            | 136        | ARG         | 2.7         |
| 47         | C            | 173        | ILE         | 2.7         |
| 1          | 1            | 2317       | C           | 2.7         |
| 1          | 1            | 3104       | C           | 2.7         |
| 1          | AS           | 3051       | C           | 2.7         |
| 46         | B            | 261        | C           | 2.7         |
| 14         | t            | 22         | VAL         | 2.7         |
| 77         | DR           | 27         | PRO         | 2.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AS    | 2313 | G    | 2.7  |
| 46  | B     | 1125 | G    | 2.7  |
| 5   | AX    | 17   | LEU  | 2.7  |
| 9   | o     | 98   | ARG  | 2.7  |
| 1   | AS    | 369  | A    | 2.7  |
| 80  | BE    | 131  | ILE  | 2.7  |
| 17  | BJ    | 122  | PRO  | 2.7  |
| 36  | CC    | 32   | LYS  | 2.7  |
| 40  | CG    | 34   | LYS  | 2.7  |
| 55  | CV    | 24   | LYS  | 2.7  |
| 7   | AZ    | 77   | ALA  | 2.7  |
| 12  | r     | 114  | GLY  | 2.7  |
| 36  | AI    | 92   | LEU  | 2.7  |
| 40  | CG    | 39   | ALA  | 2.7  |
| 48  | D     | 120  | LEU  | 2.7  |
| 1   | AS    | 882  | C    | 2.7  |
| 1   | AS    | 1781 | C    | 2.7  |
| 1   | AS    | 2745 | C    | 2.7  |
| 30  | AC    | 6    | ASN  | 2.7  |
| 41  | CH    | 43   | ASN  | 2.7  |
| 46  | B     | 1627 | C    | 2.7  |
| 53  | I     | 87   | ARG  | 2.7  |
| 7   | m     | 27   | LYS  | 2.7  |
| 50  | F     | 205  | ASP  | 2.7  |
| 8   | n     | 4    | VAL  | 2.7  |
| 54  | J     | 87   | VAL  | 2.7  |
| 1   | AS    | 776  | A    | 2.7  |
| 1   | AS    | 1127 | G    | 2.7  |
| 22  | BO    | 34   | TYR  | 2.7  |
| 54  | J     | 149  | LEU  | 2.7  |
| 70  | DK    | 119  | GLY  | 2.7  |
| 16  | v     | 203  | ARG  | 2.7  |
| 49  | E     | 213  | ILE  | 2.7  |
| 1   | 1     | 1012 | U    | 2.7  |
| 46  | B     | 1613 | U    | 2.7  |
| 33  | AF    | 27   | HIS  | 2.7  |
| 10  | BC    | 152  | VAL  | 2.7  |
| 50  | CQ    | 224  | VAL  | 2.7  |
| 1   | 1     | 3053 | C    | 2.7  |
| 17  | BJ    | 20   | LEU  | 2.7  |
| 13  | s     | 136  | ALA  | 2.7  |
| 26  | BS    | 123  | TYR  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | AH    | 16   | ARG  | 2.7  |
| 69  | Y     | 80   | ASN  | 2.7  |
| 7   | AZ    | 143  | LYS  | 2.7  |
| 20  | z     | 19   | LYS  | 2.7  |
| 18  | BK    | 88   | VAL  | 2.7  |
| 1   | 1     | 1894 | G    | 2.7  |
| 1   | AS    | 2089 | G    | 2.7  |
| 12  | r     | 171  | TRP  | 2.7  |
| 30  | BW    | 24   | PRO  | 2.7  |
| 46  | B     | 1599 | U    | 2.7  |
| 16  | v     | 50   | ARG  | 2.7  |
| 42  | AO    | 6    | ARG  | 2.7  |
| 53  | I     | 85   | ARG  | 2.7  |
| 17  | w     | 145  | ALA  | 2.7  |
| 47  | C     | 155  | TYR  | 2.7  |
| 64  | DE    | 68   | GLY  | 2.7  |
| 16  | v     | 182  | LYS  | 2.7  |
| 41  | AN    | 38   | LYS  | 2.7  |
| 42  | AO    | 16   | LYS  | 2.7  |
| 1   | 1     | 940  | C    | 2.7  |
| 1   | 1     | 1900 | C    | 2.7  |
| 46  | B     | 1013 | C    | 2.7  |
| 46  | CM    | 1619 | C    | 2.7  |
| 30  | AC    | 31   | SER  | 2.7  |
| 35  | AH    | 57   | LEU  | 2.7  |
| 17  | w     | 15   | HIS  | 2.6  |
| 71  | a     | 24   | VAL  | 2.6  |
| 14  | BG    | 85   | ILE  | 2.6  |
| 52  | CS    | 102  | ARG  | 2.6  |
| 55  | CV    | 67   | TRP  | 2.6  |
| 6   | AY    | 89   | ALA  | 2.6  |
| 7   | AZ    | 78   | ALA  | 2.6  |
| 19  | y     | 102  | ALA  | 2.6  |
| 20  | BM    | 80   | LYS  | 2.6  |
| 53  | I     | 89   | THR  | 2.6  |
| 1   | 1     | 1637 | U    | 2.6  |
| 17  | BJ    | 128  | LEU  | 2.6  |
| 75  | e     | 54   | LEU  | 2.6  |
| 46  | B     | 507  | G    | 2.6  |
| 46  | CM    | 381  | G    | 2.6  |
| 5   | k     | 4    | ARG  | 2.6  |
| 5   | k     | 252  | ILE  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | 2     | 85   | ILE  | 2.6  |
| 33  | AF    | 97   | ILE  | 2.6  |
| 4   | AW    | 229  | ALA  | 2.6  |
| 44  | AQ    | 7    | LYS  | 2.6  |
| 80  | BE    | 132  | GLY  | 2.6  |
| 1   | AS    | 1114 | C    | 2.6  |
| 1   | AS    | 1665 | C    | 2.6  |
| 9   | BB    | 127  | LEU  | 2.6  |
| 22  | BO    | 91   | LEU  | 2.6  |
| 30  | AC    | 11   | ASN  | 2.6  |
| 50  | F     | 17   | VAL  | 2.6  |
| 76  | DQ    | 6    | VAL  | 2.6  |
| 1   | AS    | 862  | A    | 2.6  |
| 13  | s     | 140  | ARG  | 2.6  |
| 7   | AZ    | 81   | HIS  | 2.6  |
| 51  | G     | 8    | HIS  | 2.6  |
| 1   | 1     | 82   | U    | 2.6  |
| 30  | AC    | 23   | LYS  | 2.6  |
| 34  | AG    | 31   | GLN  | 2.6  |
| 46  | B     | 378  | U    | 2.6  |
| 51  | CR    | 22   | LYS  | 2.6  |
| 8   | BA    | 136  | ALA  | 2.6  |
| 76  | f     | 48   | ALA  | 2.6  |
| 10  | BC    | 111  | THR  | 2.6  |
| 40  | CG    | 13   | LEU  | 2.6  |
| 50  | CQ    | 70   | LEU  | 2.6  |
| 73  | c     | 90   | THR  | 2.6  |
| 11  | BD    | 7    | ASP  | 2.6  |
| 46  | CM    | 1441 | G    | 2.6  |
| 30  | BW    | 31   | SER  | 2.6  |
| 55  | CV    | 35   | ASN  | 2.6  |
| 5   | AX    | 252  | ILE  | 2.6  |
| 19  | BL    | 140  | VAL  | 2.6  |
| 20  | z     | 22   | VAL  | 2.6  |
| 61  | Q     | 23   | VAL  | 2.6  |
| 60  | P     | 94   | LYS  | 2.6  |
| 1   | 1     | 30   | C    | 2.6  |
| 1   | 1     | 1775 | C    | 2.6  |
| 46  | B     | 1602 | C    | 2.6  |
| 14  | BG    | 86   | ALA  | 2.6  |
| 35  | AH    | 52   | ALA  | 2.6  |
| 16  | BI    | 80   | THR  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 51  | CR    | 47   | PHE  | 2.6  |
| 1   | 1     | 2675 | A    | 2.6  |
| 1   | AS    | 1584 | A    | 2.6  |
| 1   | AS    | 1879 | A    | 2.6  |
| 1   | AS    | 2431 | U    | 2.6  |
| 3   | 4     | 22   | U    | 2.6  |
| 11  | BD    | 48   | ILE  | 2.6  |
| 76  | f     | 50   | ILE  | 2.6  |
| 30  | AC    | 33   | LYS  | 2.6  |
| 55  | K     | 23   | LYS  | 2.6  |
| 63  | S     | 46   | LYS  | 2.6  |
| 6   | AY    | 90   | ALA  | 2.6  |
| 10  | p     | 201  | LEU  | 2.6  |
| 16  | BI    | 76   | PRO  | 2.6  |
| 48  | CO    | 141  | ALA  | 2.6  |
| 6   | l     | 197  | GLY  | 2.6  |
| 19  | BL    | 169  | GLY  | 2.6  |
| 70  | DK    | 48   | HIS  | 2.6  |
| 1   | 1     | 2702 | G    | 2.6  |
| 1   | AS    | 170  | G    | 2.6  |
| 18  | x     | 79   | THR  | 2.6  |
| 46  | B     | 1126 | G    | 2.6  |
| 51  | G     | 24   | SER  | 2.6  |
| 60  | P     | 84   | ILE  | 2.6  |
| 1   | 1     | 101  | C    | 2.6  |
| 1   | 1     | 2308 | C    | 2.6  |
| 1   | 1     | 2839 | C    | 2.6  |
| 32  | BY    | 22   | VAL  | 2.6  |
| 41  | CH    | 22   | LYS  | 2.6  |
| 45  | CL    | 71   | LYS  | 2.6  |
| 46  | B     | 379  | C    | 2.6  |
| 53  | I     | 157  | VAL  | 2.6  |
| 65  | U     | 44   | ASN  | 2.6  |
| 66  | DG    | 119  | LYS  | 2.6  |
| 50  | F     | 47   | LEU  | 2.6  |
| 51  | CR    | 12   | LEU  | 2.6  |
| 58  | N     | 91   | LEU  | 2.6  |
| 61  | Q     | 78   | LEU  | 2.6  |
| 63  | S     | 43   | LEU  | 2.6  |
| 1   | AS    | 1160 | A    | 2.6  |
| 37  | AJ    | 7    | ALA  | 2.6  |
| 46  | B     | 1618 | A    | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | m     | 7    | PHE  | 2.6  |
| 46  | CM    | 1613 | U    | 2.6  |
| 4   | j     | 209  | HIS  | 2.5  |
| 19  | BL    | 158  | HIS  | 2.5  |
| 5   | AX    | 337  | THR  | 2.5  |
| 4   | j     | 157  | ILE  | 2.5  |
| 50  | F     | 171  | ILE  | 2.5  |
| 6   | AY    | 48   | ARG  | 2.5  |
| 22  | BO    | 88   | ARG  | 2.5  |
| 32  | AE    | 18   | ARG  | 2.5  |
| 51  | G     | 51   | ARG  | 2.5  |
| 51  | G     | 127  | LYS  | 2.5  |
| 53  | CT    | 74   | ARG  | 2.5  |
| 63  | S     | 131  | ARG  | 2.5  |
| 5   | AX    | 73   | VAL  | 2.5  |
| 19  | BL    | 30   | VAL  | 2.5  |
| 48  | CO    | 137  | VAL  | 2.5  |
| 51  | G     | 76   | VAL  | 2.5  |
| 29  | AB    | 44   | ASN  | 2.5  |
| 22  | BO    | 151  | LEU  | 2.5  |
| 55  | K     | 96   | LEU  | 2.5  |
| 1   | AS    | 420  | G    | 2.5  |
| 4   | AW    | 210  | PRO  | 2.5  |
| 6   | AY    | 57   | ALA  | 2.5  |
| 9   | BB    | 128  | ALA  | 2.5  |
| 26  | 8     | 65   | ALA  | 2.5  |
| 46  | B     | 1115 | G    | 2.5  |
| 54  | J     | 179  | PHE  | 2.5  |
| 73  | DN    | 2    | PRO  | 2.5  |
| 53  | I     | 146  | GLY  | 2.5  |
| 62  | R     | 99   | GLY  | 2.5  |
| 3   | AU    | 21   | C    | 2.5  |
| 22  | 2     | 11   | THR  | 2.5  |
| 32  | BY    | 105  | THR  | 2.5  |
| 45  | i     | 58   | THR  | 2.5  |
| 46  | B     | 1726 | C    | 2.5  |
| 46  | CM    | 1412 | C    | 2.5  |
| 80  | BE    | 167  | ILE  | 2.5  |
| 56  | L     | 10   | LYS  | 2.5  |
| 64  | DE    | 7    | LYS  | 2.5  |
| 32  | BY    | 27   | ARG  | 2.5  |
| 49  | E     | 86   | ARG  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 60  | P     | 114  | ARG  | 2.5  |
| 47  | C     | 76   | CYS  | 2.5  |
| 56  | L     | 148  | VAL  | 2.5  |
| 62  | R     | 85   | VAL  | 2.5  |
| 1   | 1     | 155  | A    | 2.5  |
| 46  | B     | 1338 | U    | 2.5  |
| 49  | CP    | 108  | LEU  | 2.5  |
| 19  | y     | 4    | ASP  | 2.5  |
| 41  | AN    | 43   | ASN  | 2.5  |
| 62  | DC    | 89   | MET  | 2.5  |
| 13  | BF    | 144  | ALA  | 2.5  |
| 26  | 8     | 84   | PHE  | 2.5  |
| 58  | N     | 95   | PRO  | 2.5  |
| 19  | y     | 183  | GLY  | 2.5  |
| 79  | AR    | 98   | GLY  | 2.5  |
| 4   | j     | 219  | ILE  | 2.5  |
| 26  | 8     | 89   | LYS  | 2.5  |
| 61  | Q     | 110  | ILE  | 2.5  |
| 67  | DH    | 66   | THR  | 2.5  |
| 13  | s     | 51   | ARG  | 2.5  |
| 29  | AB    | 42   | ARG  | 2.5  |
| 5   | k     | 47   | LEU  | 2.5  |
| 7   | m     | 52   | VAL  | 2.5  |
| 16  | v     | 121  | VAL  | 2.5  |
| 43  | CJ    | 85   | LEU  | 2.5  |
| 49  | E     | 235  | LEU  | 2.5  |
| 53  | I     | 153  | VAL  | 2.5  |
| 53  | CT    | 161  | GLU  | 2.5  |
| 54  | J     | 178  | VAL  | 2.5  |
| 75  | e     | 48   | VAL  | 2.5  |
| 1   | 1     | 154  | G    | 2.5  |
| 1   | 1     | 1264 | G    | 2.5  |
| 1   | 1     | 1427 | G    | 2.5  |
| 1   | AS    | 219  | G    | 2.5  |
| 1   | AS    | 1440 | G    | 2.5  |
| 16  | v     | 175  | ASN  | 2.5  |
| 46  | B     | 1134 | G    | 2.5  |
| 1   | 1     | 27   | C    | 2.5  |
| 1   | AS    | 2942 | C    | 2.5  |
| 55  | CV    | 109  | PHE  | 2.5  |
| 5   | AX    | 254  | ALA  | 2.5  |
| 6   | l     | 54   | ALA  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | CN    | 132  | ALA  | 2.5  |
| 9   | BB    | 130  | PRO  | 2.5  |
| 6   | l     | 194  | LYS  | 2.5  |
| 10  | p     | 175  | GLY  | 2.5  |
| 16  | v     | 177  | GLY  | 2.5  |
| 18  | BK    | 136  | ILE  | 2.5  |
| 27  | BT    | 77   | LYS  | 2.5  |
| 34  | AG    | 30   | ILE  | 2.5  |
| 55  | K     | 41   | LYS  | 2.5  |
| 1   | AS    | 2322 | U    | 2.5  |
| 1   | AS    | 3050 | A    | 2.5  |
| 46  | B     | 1136 | A    | 2.5  |
| 46  | B     | 1400 | U    | 2.5  |
| 20  | BM    | 9    | ARG  | 2.5  |
| 73  | DN    | 89   | ARG  | 2.5  |
| 10  | p     | 153  | LEU  | 2.5  |
| 21  | 0     | 152  | LEU  | 2.5  |
| 51  | CR    | 8    | HIS  | 2.5  |
| 13  | s     | 18   | VAL  | 2.5  |
| 48  | D     | 164  | VAL  | 2.5  |
| 50  | F     | 168  | PHE  | 2.5  |
| 5   | k     | 50   | LYS  | 2.5  |
| 6   | AY    | 50   | ALA  | 2.5  |
| 16  | v     | 74   | PRO  | 2.5  |
| 26  | 8     | 67   | ILE  | 2.5  |
| 38  | AK    | 84   | LYS  | 2.5  |
| 50  | CQ    | 103  | ALA  | 2.5  |
| 15  | u     | 52   | LEU  | 2.5  |
| 33  | AF    | 34   | ARG  | 2.5  |
| 30  | AC    | 13   | THR  | 2.5  |
| 56  | L     | 49   | LEU  | 2.5  |
| 6   | AY    | 233  | HIS  | 2.5  |
| 14  | BG    | 22   | VAL  | 2.5  |
| 1   | AS    | 1185 | C    | 2.5  |
| 1   | AS    | 1489 | G    | 2.5  |
| 1   | AS    | 2936 | G    | 2.5  |
| 27  | BT    | 26   | GLU  | 2.5  |
| 29  | AB    | 63   | LYS  | 2.5  |
| 42  | CI    | 16   | LYS  | 2.5  |
| 49  | CP    | 83   | LYS  | 2.5  |
| 52  | H     | 44   | ASN  | 2.5  |
| 6   | AY    | 356  | GLN  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | m     | 151  | GLN  | 2.5  |
| 16  | v     | 55   | ALA  | 2.5  |
| 35  | CB    | 63   | ALA  | 2.5  |
| 47  | CN    | 19   | ALA  | 2.5  |
| 51  | G     | 5    | PRO  | 2.5  |
| 8   | BA    | 42   | LEU  | 2.5  |
| 48  | CO    | 120  | LEU  | 2.5  |
| 52  | CS    | 93   | LEU  | 2.5  |
| 70  | DK    | 38   | PHE  | 2.4  |
| 5   | AX    | 5    | LYS  | 2.4  |
| 75  | DP    | 45   | LYS  | 2.4  |
| 56  | CW    | 42   | ILE  | 2.4  |
| 6   | l     | 111  | ASN  | 2.4  |
| 45  | i     | 60   | ASN  | 2.4  |
| 5   | k     | 96   | PRO  | 2.4  |
| 49  | E     | 108  | LEU  | 2.4  |
| 53  | I     | 178  | LEU  | 2.4  |
| 57  | M     | 46   | LEU  | 2.4  |
| 58  | N     | 71   | LEU  | 2.4  |
| 18  | BK    | 135  | ARG  | 2.4  |
| 70  | DK    | 32   | ARG  | 2.4  |
| 73  | DN    | 31   | PRO  | 2.4  |
| 1   | 1     | 240  | C    | 2.4  |
| 1   | AS    | 944  | C    | 2.4  |
| 1   | AS    | 2852 | U    | 2.4  |
| 26  | BS    | 50   | SER  | 2.4  |
| 65  | DF    | 47   | CYS  | 2.4  |
| 1   | AS    | 215  | G    | 2.4  |
| 1   | AS    | 367  | A    | 2.4  |
| 1   | AS    | 419  | G    | 2.4  |
| 1   | AS    | 2099 | G    | 2.4  |
| 1   | AS    | 2430 | G    | 2.4  |
| 8   | BA    | 52   | VAL  | 2.4  |
| 18  | BK    | 113  | VAL  | 2.4  |
| 24  | 6     | 35   | TYR  | 2.4  |
| 36  | AI    | 83   | LYS  | 2.4  |
| 72  | DM    | 97   | LYS  | 2.4  |
| 19  | y     | 158  | HIS  | 2.4  |
| 15  | u     | 127  | ALA  | 2.4  |
| 55  | K     | 20   | GLN  | 2.4  |
| 60  | P     | 81   | ALA  | 2.4  |
| 60  | DA    | 121  | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | BI    | 78   | GLY  | 2.4  |
| 62  | DC    | 83   | MET  | 2.4  |
| 19  | BL    | 6    | THR  | 2.4  |
| 56  | CW    | 14   | VAL  | 2.4  |
| 17  | w     | 48   | PHE  | 2.4  |
| 71  | a     | 119  | PHE  | 2.4  |
| 63  | S     | 51   | LEU  | 2.4  |
| 69  | Y     | 26   | LEU  | 2.4  |
| 1   | 1     | 965  | C    | 2.4  |
| 1   | AS    | 1852 | C    | 2.4  |
| 3   | AU    | 91   | C    | 2.4  |
| 17  | BJ    | 123  | GLN  | 2.4  |
| 18  | BK    | 128  | ARG  | 2.4  |
| 35  | AH    | 3    | GLN  | 2.4  |
| 46  | B     | 695  | C    | 2.4  |
| 46  | B     | 1182 | C    | 2.4  |
| 46  | B     | 1621 | C    | 2.4  |
| 46  | B     | 1653 | U    | 2.4  |
| 52  | H     | 74   | ALA  | 2.4  |
| 56  | L     | 44   | ARG  | 2.4  |
| 56  | CW    | 3    | ARG  | 2.4  |
| 1   | 1     | 1139 | A    | 2.4  |
| 16  | v     | 86   | ASN  | 2.4  |
| 16  | BI    | 149  | ASN  | 2.4  |
| 40  | AM    | 33   | ASN  | 2.4  |
| 46  | B     | 297  | A    | 2.4  |
| 46  | B     | 383  | A    | 2.4  |
| 46  | B     | 1124 | A    | 2.4  |
| 46  | B     | 1297 | A    | 2.4  |
| 49  | E     | 76   | MET  | 2.4  |
| 73  | DN    | 20   | PRO  | 2.4  |
| 10  | p     | 183  | GLY  | 2.4  |
| 1   | 1     | 109  | G    | 2.4  |
| 6   | AY    | 105  | LYS  | 2.4  |
| 8   | BA    | 65   | SER  | 2.4  |
| 41  | CH    | 32   | THR  | 2.4  |
| 42  | CI    | 24   | SER  | 2.4  |
| 46  | B     | 750  | G    | 2.4  |
| 19  | y     | 161  | LYS  | 2.4  |
| 55  | K     | 17   | LYS  | 2.4  |
| 15  | BH    | 111  | PHE  | 2.4  |
| 19  | y     | 64   | VAL  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 78  | h     | 156  | VAL  | 2.4  |
| 4   | AW    | 208  | ASP  | 2.4  |
| 76  | f     | 55   | TYR  | 2.4  |
| 35  | AH    | 34   | HIS  | 2.4  |
| 54  | CU    | 67   | ARG  | 2.4  |
| 16  | v     | 57   | GLN  | 2.4  |
| 18  | x     | 140  | GLN  | 2.4  |
| 20  | BM    | 96   | MET  | 2.4  |
| 51  | CR    | 29   | PRO  | 2.4  |
| 6   | l     | 192  | LYS  | 2.4  |
| 11  | BD    | 27   | VAL  | 2.4  |
| 16  | BI    | 152  | VAL  | 2.4  |
| 28  | AA    | 72   | VAL  | 2.4  |
| 32  | AE    | 100  | THR  | 2.4  |
| 56  | CW    | 130  | THR  | 2.4  |
| 64  | DE    | 110  | VAL  | 2.4  |
| 68  | X     | 20   | THR  | 2.4  |
| 43  | AP    | 85   | LEU  | 2.4  |
| 48  | D     | 161  | LEU  | 2.4  |
| 59  | O     | 106  | LEU  | 2.4  |
| 1   | 1     | 26   | C    | 2.4  |
| 1   | 1     | 2745 | C    | 2.4  |
| 1   | AS    | 1487 | A    | 2.4  |
| 17  | BJ    | 82   | TYR  | 2.4  |
| 46  | CM    | 1178 | A    | 2.4  |
| 5   | k     | 74   | GLU  | 2.4  |
| 5   | AX    | 369  | ARG  | 2.4  |
| 13  | BF    | 145  | ARG  | 2.4  |
| 20  | z     | 97   | ARG  | 2.4  |
| 35  | CB    | 16   | ARG  | 2.4  |
| 41  | AN    | 37   | ARG  | 2.4  |
| 69  | Y     | 28   | ARG  | 2.4  |
| 25  | BR    | 42   | GLN  | 2.4  |
| 26  | 8     | 85   | GLN  | 2.4  |
| 32  | AE    | 31   | ALA  | 2.4  |
| 60  | DA    | 63   | ALA  | 2.4  |
| 1   | AS    | 169  | G    | 2.4  |
| 1   | AS    | 1782 | G    | 2.4  |
| 3   | AU    | 150  | G    | 2.4  |
| 46  | B     | 1339 | G    | 2.4  |
| 29  | BV    | 29   | PRO  | 2.4  |
| 53  | I     | 143  | LYS  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 56  | L     | 29   | LYS  | 2.4  |
| 43  | CJ    | 51   | GLY  | 2.4  |
| 63  | DD    | 132  | GLY  | 2.4  |
| 7   | AZ    | 142  | PHE  | 2.4  |
| 67  | W     | 75   | SER  | 2.4  |
| 71  | a     | 72   | PHE  | 2.4  |
| 7   | AZ    | 236  | VAL  | 2.4  |
| 8   | BA    | 154  | LEU  | 2.4  |
| 9   | o     | 221  | ILE  | 2.4  |
| 14  | t     | 54   | LEU  | 2.4  |
| 16  | BI    | 121  | VAL  | 2.4  |
| 32  | BY    | 92   | VAL  | 2.4  |
| 35  | CB    | 23   | VAL  | 2.4  |
| 36  | AI    | 57   | VAL  | 2.4  |
| 39  | CF    | 25   | VAL  | 2.4  |
| 63  | S     | 114  | THR  | 2.4  |
| 24  | 6     | 15   | LEU  | 2.4  |
| 58  | N     | 140  | LEU  | 2.4  |
| 16  | BI    | 26   | ARG  | 2.4  |
| 32  | BY    | 18   | ARG  | 2.4  |
| 33  | AF    | 14   | TYR  | 2.4  |
| 55  | CV    | 18   | ARG  | 2.4  |
| 77  | g     | 40   | TYR  | 2.4  |
| 16  | v     | 8    | GLU  | 2.4  |
| 49  | CP    | 87   | ALA  | 2.4  |
| 53  | I     | 91   | GLU  | 2.4  |
| 1   | AS    | 2090 | U    | 2.3  |
| 53  | CT    | 140  | HIS  | 2.3  |
| 5   | k     | 270  | ASN  | 2.3  |
| 7   | AZ    | 55   | PHE  | 2.3  |
| 9   | BB    | 94   | PRO  | 2.3  |
| 17  | BJ    | 30   | ASN  | 2.3  |
| 73  | c     | 25   | ASN  | 2.3  |
| 1   | 1     | 2350 | A    | 2.3  |
| 4   | AW    | 157  | ILE  | 2.3  |
| 6   | l     | 236  | LEU  | 2.3  |
| 46  | CM    | 40   | A    | 2.3  |
| 60  | DA    | 16   | LEU  | 2.3  |
| 61  | Q     | 97   | LEU  | 2.3  |
| 14  | t     | 63   | VAL  | 2.3  |
| 17  | w     | 9    | VAL  | 2.3  |
| 64  | DE    | 8    | THR  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | H     | 83   | ARG  | 2.3  |
| 35  | CB    | 62   | TYR  | 2.3  |
| 62  | R     | 97   | TYR  | 2.3  |
| 7   | AZ    | 34   | LYS  | 2.3  |
| 13  | s     | 168  | ASP  | 2.3  |
| 42  | AO    | 19   | LYS  | 2.3  |
| 14  | BG    | 44   | ALA  | 2.3  |
| 20  | z     | 87   | ALA  | 2.3  |
| 46  | CM    | 1452 | G    | 2.3  |
| 66  | DG    | 62   | ALA  | 2.3  |
| 71  | DL    | 88   | ALA  | 2.3  |
| 4   | AW    | 232  | GLY  | 2.3  |
| 7   | m     | 170  | GLY  | 2.3  |
| 19  | y     | 138  | LEU  | 2.3  |
| 61  | DB    | 132  | LEU  | 2.3  |
| 6   | AY    | 104  | THR  | 2.3  |
| 22  | BO    | 89   | VAL  | 2.3  |
| 62  | R     | 94   | VAL  | 2.3  |
| 73  | DN    | 29   | CYS  | 2.3  |
| 46  | B     | 492  | U    | 2.3  |
| 46  | CM    | 944  | U    | 2.3  |
| 16  | BI    | 182  | LYS  | 2.3  |
| 9   | BB    | 131  | TYR  | 2.3  |
| 20  | z     | 45   | TYR  | 2.3  |
| 1   | 1     | 1478 | A    | 2.3  |
| 1   | AS    | 652  | C    | 2.3  |
| 1   | AS    | 948  | A    | 2.3  |
| 1   | AS    | 1332 | C    | 2.3  |
| 1   | AS    | 1842 | C    | 2.3  |
| 1   | AS    | 1907 | A    | 2.3  |
| 46  | CM    | 1066 | A    | 2.3  |
| 6   | AY    | 88   | GLN  | 2.3  |
| 16  | v     | 103  | GLU  | 2.3  |
| 22  | 2     | 94   | GLU  | 2.3  |
| 71  | a     | 135  | ASP  | 2.3  |
| 27  | BT    | 20   | PHE  | 2.3  |
| 55  | K     | 27   | PHE  | 2.3  |
| 60  | P     | 80   | LEU  | 2.3  |
| 10  | p     | 67   | SER  | 2.3  |
| 50  | CQ    | 175  | HIS  | 2.3  |
| 65  | U     | 2    | PRO  | 2.3  |
| 17  | w     | 8    | VAL  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | CQ    | 17   | VAL  | 2.3  |
| 61  | DB    | 84   | THR  | 2.3  |
| 8   | n     | 7    | LYS  | 2.3  |
| 46  | B     | 1779 | G    | 2.3  |
| 33  | AF    | 30   | ALA  | 2.3  |
| 34  | CA    | 50   | ALA  | 2.3  |
| 9   | BB    | 232  | PHE  | 2.3  |
| 63  | S     | 128  | PHE  | 2.3  |
| 63  | DD    | 124  | GLU  | 2.3  |
| 69  | Y     | 14   | ILE  | 2.3  |
| 16  | v     | 198  | SER  | 2.3  |
| 25  | BR    | 38   | SER  | 2.3  |
| 40  | CG    | 50   | GLY  | 2.3  |
| 41  | AN    | 47   | PRO  | 2.3  |
| 46  | B     | 1    | U    | 2.3  |
| 46  | B     | 616  | U    | 2.3  |
| 46  | B     | 1271 | U    | 2.3  |
| 46  | CM    | 393  | U    | 2.3  |
| 6   | AY    | 59   | HIS  | 2.3  |
| 48  | CO    | 215  | VAL  | 2.3  |
| 52  | H     | 111  | VAL  | 2.3  |
| 50  | F     | 165  | THR  | 2.3  |
| 17  | BJ    | 50   | ARG  | 2.3  |
| 39  | AL    | 3    | ARG  | 2.3  |
| 46  | B     | 481  | A    | 2.3  |
| 1   | 1     | 288  | C    | 2.3  |
| 1   | 1     | 1862 | C    | 2.3  |
| 6   | AY    | 290  | LEU  | 2.3  |
| 51  | G     | 44   | LEU  | 2.3  |
| 10  | p     | 200  | ALA  | 2.3  |
| 12  | r     | 165  | ILE  | 2.3  |
| 50  | CQ    | 173  | ILE  | 2.3  |
| 53  | I     | 144  | PHE  | 2.3  |
| 55  | CV    | 21   | PHE  | 2.3  |
| 59  | O     | 101  | ALA  | 2.3  |
| 74  | d     | 26   | GLN  | 2.3  |
| 20  | BM    | 68   | GLU  | 2.3  |
| 5   | AX    | 52   | GLY  | 2.3  |
| 8   | BA    | 4    | VAL  | 2.3  |
| 27  | 9     | 95   | VAL  | 2.3  |
| 36  | AI    | 54   | VAL  | 2.3  |
| 56  | L     | 18   | PRO  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 63  | DD    | 68   | VAL  | 2.3  |
| 30  | BW    | 7    | HIS  | 2.3  |
| 58  | N     | 72   | THR  | 2.3  |
| 61  | Q     | 121  | THR  | 2.3  |
| 1   | AS    | 659  | G    | 2.3  |
| 1   | AS    | 791  | G    | 2.3  |
| 19  | y     | 52   | LEU  | 2.3  |
| 76  | f     | 36   | LEU  | 2.3  |
| 1   | AS    | 640  | U    | 2.3  |
| 1   | AS    | 870  | U    | 2.3  |
| 9   | o     | 125  | ILE  | 2.3  |
| 7   | AZ    | 151  | GLN  | 2.3  |
| 1   | 1     | 1126 | A    | 2.3  |
| 1   | AS    | 884  | A    | 2.3  |
| 11  | BD    | 33   | GLU  | 2.3  |
| 16  | v     | 171  | SER  | 2.3  |
| 35  | AH    | 79   | SER  | 2.3  |
| 46  | B     | 503  | A    | 2.3  |
| 46  | B     | 1322 | A    | 2.3  |
| 46  | CM    | 357  | A    | 2.3  |
| 1   | 1     | 2352 | C    | 2.3  |
| 1   | 1     | 2470 | C    | 2.3  |
| 1   | AS    | 165  | C    | 2.3  |
| 4   | j     | 190  | LYS  | 2.3  |
| 7   | AZ    | 52   | VAL  | 2.3  |
| 16  | v     | 58   | GLY  | 2.3  |
| 30  | AC    | 24   | PRO  | 2.3  |
| 33  | BZ    | 77   | VAL  | 2.3  |
| 46  | B     | 1783 | C    | 2.3  |
| 58  | N     | 139  | VAL  | 2.3  |
| 79  | DT    | 78   | GLY  | 2.3  |
| 7   | m     | 22   | ARG  | 2.3  |
| 16  | BI    | 172  | ARG  | 2.3  |
| 26  | 8     | 41   | THR  | 2.2  |
| 43  | CJ    | 7    | THR  | 2.2  |
| 5   | AX    | 243  | HIS  | 2.2  |
| 18  | BK    | 133  | HIS  | 2.2  |
| 33  | AF    | 21   | HIS  | 2.2  |
| 5   | k     | 324  | LEU  | 2.2  |
| 32  | AE    | 19   | LEU  | 2.2  |
| 56  | L     | 36   | LEU  | 2.2  |
| 60  | P     | 117  | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 78  | h     | 142  | LEU  | 2.2  |
| 79  | AR    | 32   | LEU  | 2.2  |
| 5   | k     | 106  | TRP  | 2.2  |
| 6   | l     | 249  | ILE  | 2.2  |
| 22  | 2     | 48   | ILE  | 2.2  |
| 14  | t     | 119  | TYR  | 2.2  |
| 52  | CS    | 170  | GLN  | 2.2  |
| 64  | DE    | 53   | TYR  | 2.2  |
| 9   | o     | 88   | LYS  | 2.2  |
| 9   | BB    | 122  | SER  | 2.2  |
| 9   | BB    | 132  | VAL  | 2.2  |
| 1   | 1     | 1134 | U    | 2.2  |
| 7   | AZ    | 15   | ARG  | 2.2  |
| 49  | CP    | 191  | VAL  | 2.2  |
| 50  | CQ    | 40   | VAL  | 2.2  |
| 70  | Z     | 4    | GLY  | 2.2  |
| 7   | m     | 59   | ASP  | 2.2  |
| 51  | CR    | 56   | LEU  | 2.2  |
| 65  | U     | 140  | THR  | 2.2  |
| 67  | W     | 69   | THR  | 2.2  |
| 79  | AR    | 101  | THR  | 2.2  |
| 8   | n     | 163  | PHE  | 2.2  |
| 10  | BC    | 76   | ILE  | 2.2  |
| 12  | r     | 199  | PHE  | 2.2  |
| 54  | J     | 88   | PHE  | 2.2  |
| 76  | DQ    | 43   | PHE  | 2.2  |
| 1   | 1     | 1089 | A    | 2.2  |
| 46  | CM    | 740  | A    | 2.2  |
| 7   | AZ    | 166  | ALA  | 2.2  |
| 24  | BQ    | 53   | ALA  | 2.2  |
| 56  | CW    | 4    | ALA  | 2.2  |
| 58  | N     | 61   | ALA  | 2.2  |
| 1   | AS    | 742  | C    | 2.2  |
| 5   | k     | 120  | LYS  | 2.2  |
| 7   | m     | 31   | TYR  | 2.2  |
| 9   | BB    | 222  | GLN  | 2.2  |
| 17  | BJ    | 54   | LYS  | 2.2  |
| 20  | BM    | 128  | LYS  | 2.2  |
| 34  | AG    | 86   | LYS  | 2.2  |
| 58  | CY    | 97   | TYR  | 2.2  |
| 66  | DG    | 84   | LYS  | 2.2  |
| 5   | AX    | 247  | ARG  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | AY    | 287  | VAL  | 2.2  |
| 24  | BQ    | 137  | VAL  | 2.2  |
| 67  | W     | 74   | GLY  | 2.2  |
| 79  | DT    | 132  | VAL  | 2.2  |
| 6   | l     | 137  | LEU  | 2.2  |
| 21  | 0     | 162  | LEU  | 2.2  |
| 24  | BQ    | 46   | LEU  | 2.2  |
| 25  | BR    | 109  | LEU  | 2.2  |
| 51  | G     | 43   | PRO  | 2.2  |
| 54  | CU    | 95   | LEU  | 2.2  |
| 7   | m     | 60   | ILE  | 2.2  |
| 22  | BO    | 75   | ILE  | 2.2  |
| 44  | CK    | 14   | PHE  | 2.2  |
| 6   | AY    | 243  | ALA  | 2.2  |
| 7   | AZ    | 134  | ALA  | 2.2  |
| 15  | u     | 126  | LYS  | 2.2  |
| 16  | v     | 79   | ALA  | 2.2  |
| 29  | AB    | 69   | TRP  | 2.2  |
| 38  | AK    | 41   | ALA  | 2.2  |
| 46  | B     | 1064 | U    | 2.2  |
| 47  | C     | 14   | ALA  | 2.2  |
| 15  | u     | 119  | GLN  | 2.2  |
| 47  | CN    | 137  | SER  | 2.2  |
| 51  | G     | 149  | TYR  | 2.2  |
| 1   | 1     | 2453 | G    | 2.2  |
| 1   | AS    | 1893 | G    | 2.2  |
| 16  | v     | 105  | ARG  | 2.2  |
| 19  | BL    | 26   | LEU  | 2.2  |
| 19  | BL    | 29   | LEU  | 2.2  |
| 52  | CS    | 194  | LEU  | 2.2  |
| 62  | DC    | 86   | VAL  | 2.2  |
| 73  | DN    | 14   | GLY  | 2.2  |
| 1   | AS    | 2259 | A    | 2.2  |
| 46  | B     | 1407 | A    | 2.2  |
| 46  | CM    | 1078 | A    | 2.2  |
| 46  | CM    | 1403 | A    | 2.2  |
| 56  | L     | 147  | THR  | 2.2  |
| 71  | a     | 25   | ILE  | 2.2  |
| 7   | m     | 20   | PHE  | 2.2  |
| 1   | 1     | 639  | C    | 2.2  |
| 1   | AS    | 864  | C    | 2.2  |
| 1   | AS    | 2315 | C    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 16  | v     | 195  | ASN  | 2.2  |
| 46  | CM    | 1318 | C    | 2.2  |
| 10  | p     | 207  | ALA  | 2.2  |
| 51  | CR    | 13   | ALA  | 2.2  |
| 55  | K     | 204  | ALA  | 2.2  |
| 70  | Z     | 25   | ALA  | 2.2  |
| 7   | m     | 50   | ARG  | 2.2  |
| 9   | BB    | 104  | LEU  | 2.2  |
| 18  | x     | 20   | SER  | 2.2  |
| 56  | CW    | 13   | SER  | 2.2  |
| 57  | M     | 51   | SER  | 2.2  |
| 35  | AH    | 41   | ARG  | 2.2  |
| 66  | V     | 86   | ARG  | 2.2  |
| 6   | AY    | 360  | VAL  | 2.2  |
| 35  | CB    | 65   | VAL  | 2.2  |
| 24  | 6     | 20   | GLY  | 2.2  |
| 33  | AF    | 31   | GLU  | 2.2  |
| 9   | BB    | 93   | ILE  | 2.2  |
| 20  | BM    | 15   | ILE  | 2.2  |
| 34  | AG    | 100  | ILE  | 2.2  |
| 78  | h     | 133  | ILE  | 2.2  |
| 1   | 1     | 825  | U    | 2.2  |
| 1   | AS    | 167  | U    | 2.2  |
| 1   | AS    | 2926 | U    | 2.2  |
| 9   | BB    | 107  | THR  | 2.2  |
| 46  | B     | 778  | U    | 2.2  |
| 46  | B     | 779  | U    | 2.2  |
| 46  | CM    | 1673 | U    | 2.2  |
| 55  | K     | 62   | THR  | 2.2  |
| 30  | BW    | 23   | LYS  | 2.2  |
| 38  | AK    | 52   | LYS  | 2.2  |
| 16  | BI    | 90   | ASN  | 2.2  |
| 15  | u     | 34   | ASP  | 2.2  |
| 59  | O     | 120  | CYS  | 2.2  |
| 1   | 1     | 1895 | G    | 2.2  |
| 1   | AS    | 879  | A    | 2.2  |
| 1   | AS    | 1020 | G    | 2.2  |
| 1   | AS    | 1478 | A    | 2.2  |
| 12  | r     | 59   | GLN  | 2.2  |
| 14  | t     | 19   | GLN  | 2.2  |
| 27  | 9     | 30   | LEU  | 2.2  |
| 50  | CQ    | 73   | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 64  | DE    | 42   | GLN  | 2.2  |
| 74  | d     | 21   | LEU  | 2.2  |
| 52  | CS    | 112  | ARG  | 2.2  |
| 9   | BB    | 134  | TYR  | 2.2  |
| 26  | 8     | 83   | VAL  | 2.2  |
| 48  | D     | 121  | VAL  | 2.2  |
| 55  | CV    | 172  | TYR  | 2.2  |
| 1   | 1     | 1332 | C    | 2.2  |
| 1   | AS    | 172  | C    | 2.2  |
| 6   | l     | 58   | GLY  | 2.2  |
| 33  | BZ    | 52   | PRO  | 2.2  |
| 46  | B     | 1612 | C    | 2.2  |
| 80  | BE    | 149  | ILE  | 2.2  |
| 4   | j     | 16   | PHE  | 2.2  |
| 26  | 8     | 52   | PRO  | 2.2  |
| 20  | z     | 21   | LYS  | 2.2  |
| 52  | H     | 147  | THR  | 2.2  |
| 55  | CV    | 23   | LYS  | 2.2  |
| 6   | AY    | 195  | LEU  | 2.2  |
| 7   | m     | 131  | LEU  | 2.2  |
| 13  | BF    | 134  | ALA  | 2.1  |
| 60  | DA    | 22   | ALA  | 2.1  |
| 26  | BS    | 48   | ARG  | 2.1  |
| 6   | l     | 281  | ILE  | 2.1  |
| 17  | w     | 119  | VAL  | 2.1  |
| 47  | C     | 75   | VAL  | 2.1  |
| 63  | DD    | 38   | VAL  | 2.1  |
| 5   | k     | 236  | LYS  | 2.1  |
| 33  | AF    | 9    | LYS  | 2.1  |
| 33  | BZ    | 31   | GLU  | 2.1  |
| 50  | F     | 149  | LYS  | 2.1  |
| 67  | W     | 66   | THR  | 2.1  |
| 1   | 1     | 99   | A    | 2.1  |
| 46  | B     | 1011 | A    | 2.1  |
| 46  | CM    | 1574 | A    | 2.1  |
| 1   | AS    | 245  | G    | 2.1  |
| 1   | AS    | 1130 | G    | 2.1  |
| 13  | BF    | 80   | LEU  | 2.1  |
| 32  | BY    | 19   | LEU  | 2.1  |
| 52  | H     | 108  | LEU  | 2.1  |
| 25  | BR    | 125  | ALA  | 2.1  |
| 14  | t     | 21   | ARG  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1     | 1552 | C    | 2.1  |
| 1   | 1     | 2698 | C    | 2.1  |
| 1   | AS    | 934  | C    | 2.1  |
| 1   | AS    | 2545 | C    | 2.1  |
| 27  | BT    | 11   | SER  | 2.1  |
| 52  | CS    | 152  | SER  | 2.1  |
| 30  | BW    | 10   | HIS  | 2.1  |
| 30  | BW    | 48   | HIS  | 2.1  |
| 14  | t     | 93   | ILE  | 2.1  |
| 62  | R     | 84   | ILE  | 2.1  |
| 29  | BV    | 79   | TRP  | 2.1  |
| 17  | w     | 52   | LYS  | 2.1  |
| 35  | AH    | 67   | LYS  | 2.1  |
| 50  | CQ    | 188  | LYS  | 2.1  |
| 55  | K     | 109  | PHE  | 2.1  |
| 7   | m     | 26   | GLY  | 2.1  |
| 26  | BS    | 116  | PRO  | 2.1  |
| 64  | T     | 55   | THR  | 2.1  |
| 1   | 1     | 1327 | U    | 2.1  |
| 4   | AW    | 179  | LEU  | 2.1  |
| 46  | B     | 493  | U    | 2.1  |
| 46  | B     | 1393 | U    | 2.1  |
| 46  | B     | 1652 | U    | 2.1  |
| 46  | CM    | 1267 | U    | 2.1  |
| 51  | G     | 56   | LEU  | 2.1  |
| 51  | CR    | 38   | LEU  | 2.1  |
| 58  | N     | 5    | LEU  | 2.1  |
| 63  | DD    | 43   | LEU  | 2.1  |
| 81  | P0    | 15   | LEU  | 2.1  |
| 8   | BA    | 144  | ALA  | 2.1  |
| 59  | O     | 111  | ASN  | 2.1  |
| 79  | DT    | 28   | ALA  | 2.1  |
| 16  | v     | 204  | SER  | 2.1  |
| 34  | AG    | 15   | SER  | 2.1  |
| 54  | J     | 146  | GLN  | 2.1  |
| 16  | BI    | 194  | HIS  | 2.1  |
| 1   | 1     | 966  | A    | 2.1  |
| 24  | 6     | 89   | ASP  | 2.1  |
| 28  | AA    | 118  | PHE  | 2.1  |
| 70  | Z     | 3    | LYS  | 2.1  |
| 71  | DL    | 72   | PHE  | 2.1  |
| 5   | AX    | 253  | GLY  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 37         | AJ           | 65         | GLU         | 2.1         |
| 1          | AS           | 595        | G           | 2.1         |
| 4          | AW           | 249        | THR         | 2.1         |
| 48         | CO           | 46         | THR         | 2.1         |
| 62         | DC           | 11         | THR         | 2.1         |
| 78         | h            | 129        | THR         | 2.1         |
| 1          | 1            | 242        | C           | 2.1         |
| 1          | AS           | 639        | C           | 2.1         |
| 1          | AS           | 3065       | C           | 2.1         |
| 46         | CM           | 1264       | C           | 2.1         |
| 46         | CM           | 1626       | C           | 2.1         |
| 4          | j            | 115        | ASN         | 2.1         |
| 4          | AW           | 226        | SER         | 2.1         |
| 6          | AY           | 329        | ASN         | 2.1         |
| 19         | y            | 67         | ILE         | 2.1         |
| 53         | CT           | 78         | SER         | 2.1         |
| 56         | CW           | 45         | ILE         | 2.1         |
| 4          | j            | 234        | LYS         | 2.1         |
| 14         | BG           | 16         | LYS         | 2.1         |
| 16         | BI           | 96         | LYS         | 2.1         |
| 43         | AP           | 53         | GLN         | 2.1         |
| 45         | i            | 100        | LYS         | 2.1         |
| 1          | 1            | 153        | U           | 2.1         |
| 1          | 1            | 641        | U           | 2.1         |
| 1          | AS           | 2366       | U           | 2.1         |
| 20         | BM           | 51         | VAL         | 2.1         |
| 32         | BY           | 66         | VAL         | 2.1         |
| 46         | B            | 1569       | U           | 2.1         |
| 46         | CM           | 1129       | U           | 2.1         |
| 65         | DF           | 70         | VAL         | 2.1         |
| 30         | AC           | 7          | HIS         | 2.1         |
| 76         | DQ           | 3          | HIS         | 2.1         |
| 51         | G            | 23         | LEU         | 2.1         |
| 5          | k            | 19         | ARG         | 2.1         |
| 55         | CV           | 77         | ARG         | 2.1         |
| 67         | W            | 67         | ARG         | 2.1         |
| 1          | 1            | 2699       | A           | 2.1         |
| 1          | AS           | 2362       | A           | 2.1         |
| 1          | AS           | 2966       | A           | 2.1         |
| 8          | BA           | 132        | ALA         | 2.1         |
| 46         | B            | 619        | A           | 2.1         |
| 46         | B            | 1316       | A           | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | B     | 1403 | A    | 2.1  |
| 52  | CS    | 190  | ILE  | 2.1  |
| 19  | BL    | 185  | LYS  | 2.1  |
| 29  | BV    | 10   | LYS  | 2.1  |
| 68  | DI    | 25   | LYS  | 2.1  |
| 32  | AE    | 38   | PHE  | 2.1  |
| 34  | AG    | 85   | PHE  | 2.1  |
| 55  | CV    | 27   | PHE  | 2.1  |
| 70  | DK    | 122  | PHE  | 2.1  |
| 71  | a     | 122  | GLN  | 2.1  |
| 4   | AW    | 202  | VAL  | 2.1  |
| 6   | AY    | 43   | VAL  | 2.1  |
| 20  | BM    | 17   | VAL  | 2.1  |
| 5   | k     | 17   | LEU  | 2.1  |
| 1   | AS    | 1352 | C    | 2.1  |
| 1   | AS    | 1777 | C    | 2.1  |
| 1   | AS    | 2321 | C    | 2.1  |
| 1   | AS    | 175  | G    | 2.1  |
| 1   | AS    | 1660 | G    | 2.1  |
| 1   | AS    | 2579 | G    | 2.1  |
| 1   | AS    | 2580 | G    | 2.1  |
| 1   | AS    | 2582 | G    | 2.1  |
| 9   | BB    | 136  | TYR  | 2.1  |
| 35  | CB    | 7    | TYR  | 2.1  |
| 45  | CL    | 111  | ASP  | 2.1  |
| 46  | CM    | 1135 | G    | 2.1  |
| 70  | Z     | 2    | GLY  | 2.1  |
| 18  | x     | 123  | PRO  | 2.1  |
| 57  | M     | 96   | PRO  | 2.1  |
| 77  | g     | 30   | PRO  | 2.1  |
| 5   | k     | 276  | THR  | 2.1  |
| 64  | T     | 106  | THR  | 2.1  |
| 51  | CR    | 11   | ARG  | 2.1  |
| 16  | v     | 56   | LYS  | 2.1  |
| 46  | CM    | 1399 | U    | 2.1  |
| 61  | Q     | 76   | ILE  | 2.1  |
| 6   | AY    | 71   | ALA  | 2.1  |
| 11  | BD    | 52   | ALA  | 2.1  |
| 13  | BF    | 136  | ALA  | 2.1  |
| 16  | BI    | 3    | ALA  | 2.1  |
| 54  | CU    | 55   | ALA  | 2.1  |
| 62  | DC    | 74   | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | BB    | 102  | GLN  | 2.1  |
| 66  | V     | 14   | PHE  | 2.1  |
| 26  | BS    | 83   | VAL  | 2.1  |
| 51  | G     | 157  | ASN  | 2.1  |
| 75  | e     | 51   | ASN  | 2.1  |
| 62  | R     | 80   | LEU  | 2.1  |
| 1   | AS    | 988  | A    | 2.0  |
| 1   | AS    | 1892 | A    | 2.0  |
| 5   | AX    | 274  | HIS  | 2.0  |
| 16  | v     | 81   | TYR  | 2.0  |
| 22  | 2     | 56   | TYR  | 2.0  |
| 35  | AH    | 78   | GLY  | 2.0  |
| 61  | Q     | 108  | GLY  | 2.0  |
| 16  | v     | 187  | ARG  | 2.0  |
| 20  | BM    | 97   | ARG  | 2.0  |
| 4   | AW    | 77   | ILE  | 2.0  |
| 5   | k     | 227  | GLU  | 2.0  |
| 5   | AX    | 24   | LYS  | 2.0  |
| 6   | AY    | 281  | ILE  | 2.0  |
| 4   | j     | 235  | ALA  | 2.0  |
| 10  | p     | 179  | ALA  | 2.0  |
| 38  | AK    | 65   | ALA  | 2.0  |
| 45  | i     | 51   | ALA  | 2.0  |
| 52  | H     | 79   | SER  | 2.0  |
| 65  | U     | 58   | ALA  | 2.0  |
| 1   | 1     | 332  | C    | 2.0  |
| 6   | AY    | 236  | LEU  | 2.0  |
| 17  | BJ    | 100  | LEU  | 2.0  |
| 46  | CM    | 1627 | C    | 2.0  |
| 47  | C     | 177  | LEU  | 2.0  |
| 55  | K     | 185  | CYS  | 2.0  |
| 59  | CZ    | 103  | LEU  | 2.0  |
| 64  | T     | 109  | LEU  | 2.0  |
| 7   | m     | 105  | VAL  | 2.0  |
| 28  | AA    | 24   | VAL  | 2.0  |
| 63  | S     | 47   | VAL  | 2.0  |
| 71  | a     | 126  | GLN  | 2.0  |
| 35  | CB    | 14   | ASN  | 2.0  |
| 1   | 1     | 103  | G    | 2.0  |
| 1   | 1     | 333  | G    | 2.0  |
| 1   | 1     | 1159 | G    | 2.0  |
| 1   | AS    | 2965 | G    | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | AS    | 3031 | G    | 2.0  |
| 1   | AS    | 631  | U    | 2.0  |
| 1   | AS    | 2925 | U    | 2.0  |
| 29  | BV    | 109  | TYR  | 2.0  |
| 8   | BA    | 139  | LYS  | 2.0  |
| 52  | H     | 72   | HIS  | 2.0  |
| 20  | z     | 15   | ILE  | 2.0  |
| 56  | L     | 120  | ARG  | 2.0  |
| 30  | BW    | 8    | THR  | 2.0  |
| 64  | T     | 8    | THR  | 2.0  |
| 75  | e     | 53   | ILE  | 2.0  |
| 4   | j     | 96   | LEU  | 2.0  |
| 5   | k     | 267  | ALA  | 2.0  |
| 9   | o     | 236  | LEU  | 2.0  |
| 9   | BB    | 214  | ALA  | 2.0  |
| 58  | N     | 42   | PHE  | 2.0  |
| 17  | w     | 100  | LEU  | 2.0  |
| 59  | O     | 49   | SER  | 2.0  |
| 63  | S     | 133  | ALA  | 2.0  |
| 1   | 1     | 107  | A    | 2.0  |
| 1   | 1     | 2097 | A    | 2.0  |
| 1   | AS    | 70   | A    | 2.0  |
| 46  | B     | 1015 | A    | 2.0  |
| 46  | B     | 1321 | A    | 2.0  |
| 49  | CP    | 178  | VAL  | 2.0  |
| 50  | F     | 187  | VAL  | 2.0  |
| 16  | BI    | 117  | ASN  | 2.0  |
| 9   | BB    | 223  | GLY  | 2.0  |
| 14  | t     | 64   | LYS  | 2.0  |
| 32  | AE    | 36   | LYS  | 2.0  |
| 33  | BZ    | 49   | GLY  | 2.0  |
| 49  | CP    | 155  | GLY  | 2.0  |
| 5   | k     | 256  | HIS  | 2.0  |
| 7   | m     | 38   | THR  | 2.0  |
| 46  | CM    | 25   | C    | 2.0  |
| 46  | CM    | 695  | C    | 2.0  |
| 8   | n     | 169  | ASP  | 2.0  |
| 10  | BC    | 167  | LEU  | 2.0  |
| 19  | y     | 104  | LEU  | 2.0  |
| 56  | L     | 33   | GLU  | 2.0  |
| 56  | L     | 128  | LEU  | 2.0  |
| 57  | M     | 98   | GLU  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 80  | BE    | 57   | LEU  | 2.0  |
| 1   | 1     | 1091 | U    | 2.0  |
| 1   | 1     | 2697 | U    | 2.0  |
| 1   | 1     | 2950 | U    | 2.0  |
| 1   | 1     | 2968 | U    | 2.0  |
| 4   | AW    | 185  | ALA  | 2.0  |
| 35  | AH    | 82   | ALA  | 2.0  |
| 46  | CM    | 94   | U    | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 84  | MG   | AS    | 3650 | 1/1   | 0.08 | 0.09 | 115,115,115,115            | 0     |
| 84  | MG   | BL    | 202  | 1/1   | 0.09 | 0.24 | 107,107,107,107            | 0     |
| 84  | MG   | 1     | 3751 | 1/1   | 0.10 | 0.26 | 111,111,111,111            | 0     |
| 84  | MG   | B     | 1886 | 1/1   | 0.27 | 0.13 | 66,66,66,66                | 0     |
| 84  | MG   | AS    | 3517 | 1/1   | 0.28 | 0.25 | 106,106,106,106            | 0     |
| 84  | MG   | AS    | 3536 | 1/1   | 0.28 | 0.34 | 110,110,110,110            | 0     |
| 84  | MG   | BC    | 301  | 1/1   | 0.29 | 0.32 | 125,125,125,125            | 0     |
| 84  | MG   | AS    | 3715 | 1/1   | 0.32 | 0.31 | 158,158,158,158            | 0     |
| 84  | MG   | AS    | 3713 | 1/1   | 0.33 | 0.25 | 95,95,95,95                | 0     |
| 84  | MG   | 1     | 3570 | 1/1   | 0.34 | 0.22 | 112,112,112,112            | 0     |
| 84  | MG   | AS    | 3576 | 1/1   | 0.35 | 0.20 | 97,97,97,97                | 0     |
| 84  | MG   | AS    | 3641 | 1/1   | 0.36 | 1.19 | 81,81,81,81                | 0     |
| 84  | MG   | 1     | 3778 | 1/1   | 0.36 | 0.24 | 80,80,80,80                | 0     |
| 84  | MG   | AS    | 3756 | 1/1   | 0.37 | 0.20 | 69,69,69,69                | 0     |
| 84  | MG   | 1     | 3726 | 1/1   | 0.39 | 0.13 | 96,96,96,96                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3649 | 1/1   | 0.39 | 0.17 | 101,101,101,101             | 0     |
| 84  | MG   | 1     | 3837 | 1/1   | 0.39 | 0.24 | 82,82,82,82                 | 0     |
| 84  | MG   | 1     | 3595 | 1/1   | 0.39 | 0.30 | 89,89,89,89                 | 0     |
| 84  | MG   | AS    | 3692 | 1/1   | 0.41 | 0.18 | 86,86,86,86                 | 0     |
| 84  | MG   | CM    | 1830 | 1/1   | 0.41 | 0.24 | 96,96,96,96                 | 0     |
| 84  | MG   | 1     | 3761 | 1/1   | 0.42 | 0.31 | 106,106,106,106             | 0     |
| 84  | MG   | AS    | 3765 | 1/1   | 0.43 | 0.22 | 96,96,96,96                 | 0     |
| 84  | MG   | 1     | 3800 | 1/1   | 0.43 | 0.11 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3489 | 1/1   | 0.44 | 0.34 | 57,57,57,57                 | 0     |
| 84  | MG   | 1     | 3481 | 1/1   | 0.44 | 0.39 | 113,113,113,113             | 0     |
| 84  | MG   | 1     | 3770 | 1/1   | 0.44 | 0.22 | 85,85,85,85                 | 0     |
| 84  | MG   | AS    | 3585 | 1/1   | 0.45 | 0.27 | 78,78,78,78                 | 0     |
| 84  | MG   | AS    | 3716 | 1/1   | 0.47 | 0.19 | 86,86,86,86                 | 0     |
| 84  | MG   | AS    | 3560 | 1/1   | 0.47 | 0.32 | 96,96,96,96                 | 0     |
| 84  | MG   | DK    | 201  | 1/1   | 0.47 | 0.16 | 91,91,91,91                 | 0     |
| 84  | MG   | AS    | 3703 | 1/1   | 0.48 | 0.15 | 77,77,77,77                 | 0     |
| 84  | MG   | o     | 304  | 1/1   | 0.48 | 0.17 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3870 | 1/1   | 0.49 | 0.43 | 87,87,87,87                 | 0     |
| 84  | MG   | 1     | 3741 | 1/1   | 0.49 | 0.25 | 98,98,98,98                 | 0     |
| 84  | MG   | 1     | 3747 | 1/1   | 0.49 | 0.28 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3651 | 1/1   | 0.49 | 0.17 | 122,122,122,122             | 0     |
| 84  | MG   | AS    | 3678 | 1/1   | 0.49 | 0.17 | 108,108,108,108             | 0     |
| 84  | MG   | AS    | 3735 | 1/1   | 0.49 | 0.24 | 89,89,89,89                 | 0     |
| 84  | MG   | AS    | 3673 | 1/1   | 0.50 | 0.14 | 79,79,79,79                 | 0     |
| 84  | MG   | AS    | 3752 | 1/1   | 0.50 | 0.21 | 115,115,115,115             | 0     |
| 84  | MG   | 1     | 3756 | 1/1   | 0.51 | 0.15 | 79,79,79,79                 | 0     |
| 84  | MG   | B     | 1803 | 1/1   | 0.51 | 0.26 | 113,113,113,113             | 0     |
| 84  | MG   | AY    | 402  | 1/1   | 0.52 | 0.19 | 120,120,120,120             | 0     |
| 84  | MG   | AS    | 3614 | 1/1   | 0.52 | 0.12 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3569 | 1/1   | 0.52 | 0.27 | 89,89,89,89                 | 0     |
| 84  | MG   | 1     | 3567 | 1/1   | 0.52 | 0.25 | 87,87,87,87                 | 0     |
| 84  | MG   | CM    | 1878 | 1/1   | 0.52 | 0.11 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3481 | 1/1   | 0.52 | 0.29 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3711 | 1/1   | 0.53 | 0.17 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3505 | 1/1   | 0.53 | 0.16 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3710 | 1/1   | 0.53 | 0.20 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3408 | 1/1   | 0.53 | 0.17 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3441 | 1/1   | 0.54 | 0.32 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3605 | 1/1   | 0.54 | 0.17 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3799 | 1/1   | 0.54 | 0.10 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3576 | 1/1   | 0.54 | 0.16 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3518 | 1/1   | 0.55 | 0.23 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3529 | 1/1   | 0.55 | 0.12 | 88,88,88,88                 | 0     |
| 84  | MG   | 1     | 3423 | 1/1   | 0.55 | 0.22 | 103,103,103,103             | 0     |
| 84  | MG   | 1     | 3675 | 1/1   | 0.56 | 0.26 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3588 | 1/1   | 0.56 | 0.28 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3476 | 1/1   | 0.56 | 0.25 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3789 | 1/1   | 0.56 | 0.14 | 94,94,94,94                 | 0     |
| 84  | MG   | AS    | 3580 | 1/1   | 0.56 | 0.13 | 80,80,80,80                 | 0     |
| 84  | MG   | B     | 1850 | 1/1   | 0.57 | 0.26 | 198,198,198,198             | 0     |
| 84  | MG   | 1     | 3508 | 1/1   | 0.57 | 0.60 | 123,123,123,123             | 0     |
| 84  | MG   | CL    | 301  | 1/1   | 0.57 | 0.49 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3662 | 1/1   | 0.57 | 0.12 | 88,88,88,88                 | 0     |
| 84  | MG   | AS    | 3729 | 1/1   | 0.57 | 0.12 | 71,71,71,71                 | 0     |
| 84  | MG   | B     | 1834 | 1/1   | 0.57 | 0.23 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3754 | 1/1   | 0.58 | 0.16 | 108,108,108,108             | 0     |
| 84  | MG   | C     | 301  | 1/1   | 0.58 | 0.10 | 89,89,89,89                 | 0     |
| 84  | MG   | 1     | 3824 | 1/1   | 0.58 | 0.20 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3755 | 1/1   | 0.58 | 0.15 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3415 | 1/1   | 0.58 | 0.15 | 69,69,69,69                 | 0     |
| 84  | MG   | AS    | 3601 | 1/1   | 0.58 | 0.23 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3492 | 1/1   | 0.58 | 0.32 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3723 | 1/1   | 0.59 | 0.28 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3742 | 1/1   | 0.59 | 0.15 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3678 | 1/1   | 0.59 | 0.21 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3730 | 1/1   | 0.59 | 0.32 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3776 | 1/1   | 0.59 | 0.27 | 66,66,66,66                 | 0     |
| 84  | MG   | B     | 1859 | 1/1   | 0.59 | 0.23 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3490 | 1/1   | 0.60 | 0.24 | 47,47,47,47                 | 0     |
| 84  | MG   | 1     | 3744 | 1/1   | 0.60 | 0.16 | 84,84,84,84                 | 0     |
| 84  | MG   | B     | 1821 | 1/1   | 0.60 | 0.24 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3722 | 1/1   | 0.60 | 0.12 | 82,82,82,82                 | 0     |
| 84  | MG   | 1     | 3785 | 1/1   | 0.61 | 0.21 | 35,35,35,35                 | 0     |
| 84  | MG   | 1     | 3731 | 1/1   | 0.61 | 0.45 | 82,82,82,82                 | 0     |
| 84  | MG   | 1     | 3470 | 1/1   | 0.61 | 0.25 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3618 | 1/1   | 0.61 | 0.17 | 73,73,73,73                 | 0     |
| 84  | MG   | 1     | 3593 | 1/1   | 0.61 | 0.23 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3539 | 1/1   | 0.61 | 0.23 | 95,95,95,95                 | 0     |
| 84  | MG   | AS    | 3584 | 1/1   | 0.62 | 0.19 | 99,99,99,99                 | 0     |
| 84  | MG   | 1     | 3405 | 1/1   | 0.62 | 0.22 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3665 | 1/1   | 0.62 | 0.20 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3698 | 1/1   | 0.62 | 0.20 | 79,79,79,79                 | 0     |
| 84  | MG   | 1     | 3825 | 1/1   | 0.62 | 0.18 | 104,104,104,104             | 0     |
| 84  | MG   | 1     | 3794 | 1/1   | 0.62 | 0.13 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3717 | 1/1   | 0.62 | 0.30 | 79,79,79,79                 | 0     |
| 84  | MG   | AS    | 3674 | 1/1   | 0.63 | 0.10 | 94,94,94,94                 | 0     |
| 84  | MG   | AS    | 3568 | 1/1   | 0.63 | 0.20 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3790 | 1/1   | 0.63 | 0.24 | 98,98,98,98                 | 0     |
| 84  | MG   | 1     | 3787 | 1/1   | 0.63 | 0.11 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3821 | 1/1   | 0.63 | 0.17 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3739 | 1/1   | 0.63 | 0.34 | 93,93,93,93                 | 0     |
| 84  | MG   | CG    | 101  | 1/1   | 0.63 | 0.14 | 101,101,101,101             | 0     |
| 84  | MG   | AS    | 3751 | 1/1   | 0.63 | 0.13 | 81,81,81,81                 | 0     |
| 84  | MG   | 3     | 206  | 1/1   | 0.63 | 0.20 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3663 | 1/1   | 0.63 | 0.17 | 103,103,103,103             | 0     |
| 84  | MG   | AS    | 3525 | 1/1   | 0.63 | 0.16 | 46,46,46,46                 | 0     |
| 84  | MG   | AS    | 3759 | 1/1   | 0.64 | 0.29 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3662 | 1/1   | 0.64 | 0.17 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3823 | 1/1   | 0.64 | 0.14 | 99,99,99,99                 | 0     |
| 84  | MG   | 1     | 3451 | 1/1   | 0.64 | 0.13 | 50,50,50,50                 | 0     |
| 84  | MG   | AS    | 3512 | 1/1   | 0.64 | 0.27 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3543 | 1/1   | 0.64 | 0.21 | 58,58,58,58                 | 0     |
| 84  | MG   | 1     | 3599 | 1/1   | 0.64 | 0.13 | 72,72,72,72                 | 0     |
| 84  | MG   | AS    | 3744 | 1/1   | 0.64 | 0.29 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3547 | 1/1   | 0.64 | 0.19 | 72,72,72,72                 | 0     |
| 84  | MG   | AS    | 3709 | 1/1   | 0.64 | 0.06 | 90,90,90,90                 | 0     |
| 84  | MG   | 1     | 3681 | 1/1   | 0.64 | 0.15 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3689 | 1/1   | 0.64 | 0.22 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3733 | 1/1   | 0.65 | 0.38 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3433 | 1/1   | 0.65 | 0.23 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3740 | 1/1   | 0.65 | 0.22 | 79,79,79,79                 | 0     |
| 84  | MG   | CM    | 1826 | 1/1   | 0.65 | 0.15 | 69,69,69,69                 | 0     |
| 84  | MG   | AS    | 3705 | 1/1   | 0.65 | 0.23 | 78,78,78,78                 | 0     |
| 84  | MG   | CM    | 1850 | 1/1   | 0.65 | 0.15 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3697 | 1/1   | 0.65 | 0.16 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3691 | 1/1   | 0.65 | 0.10 | 73,73,73,73                 | 0     |
| 84  | MG   | AS    | 3783 | 1/1   | 0.66 | 0.20 | 84,84,84,84                 | 0     |
| 84  | MG   | 1     | 3585 | 1/1   | 0.66 | 0.18 | 98,98,98,98                 | 0     |
| 84  | MG   | 1     | 3546 | 1/1   | 0.66 | 0.14 | 82,82,82,82                 | 0     |
| 84  | MG   | 1     | 3841 | 1/1   | 0.66 | 0.15 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3511 | 1/1   | 0.66 | 0.20 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3417 | 1/1   | 0.66 | 0.24 | 82,82,82,82                 | 0     |
| 84  | MG   | 1     | 3788 | 1/1   | 0.66 | 0.23 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3565 | 1/1   | 0.66 | 0.11 | 49,49,49,49                 | 0     |
| 84  | MG   | CM    | 1816 | 1/1   | 0.66 | 0.24 | 67,67,67,67                 | 0     |
| 84  | MG   | B     | 1900 | 1/1   | 0.66 | 0.18 | 101,101,101,101             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3714 | 1/1   | 0.66 | 0.20 | 54,54,54,54                 | 0     |
| 84  | MG   | B     | 1802 | 1/1   | 0.66 | 0.25 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3764 | 1/1   | 0.66 | 0.12 | 86,86,86,86                 | 0     |
| 84  | MG   | DG    | 201  | 1/1   | 0.66 | 0.16 | 121,121,121,121             | 0     |
| 84  | MG   | AS    | 3532 | 1/1   | 0.66 | 0.31 | 65,65,65,65                 | 0     |
| 84  | MG   | AS    | 3542 | 1/1   | 0.67 | 0.28 | 61,61,61,61                 | 0     |
| 84  | MG   | AX    | 401  | 1/1   | 0.67 | 0.08 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3768 | 1/1   | 0.67 | 0.10 | 62,62,62,62                 | 0     |
| 84  | MG   | CM    | 1846 | 1/1   | 0.67 | 0.23 | 69,69,69,69                 | 0     |
| 84  | MG   | CM    | 1847 | 1/1   | 0.67 | 0.17 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3535 | 1/1   | 0.67 | 0.27 | 86,86,86,86                 | 0     |
| 84  | MG   | CM    | 1871 | 1/1   | 0.67 | 0.20 | 76,76,76,76                 | 0     |
| 84  | MG   | AS    | 3720 | 1/1   | 0.67 | 0.19 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3721 | 1/1   | 0.67 | 0.11 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3633 | 1/1   | 0.67 | 0.27 | 43,43,43,43                 | 0     |
| 84  | MG   | B     | 1885 | 1/1   | 0.68 | 0.15 | 100,100,100,100             | 0     |
| 84  | MG   | 1     | 3732 | 1/1   | 0.68 | 0.28 | 65,65,65,65                 | 0     |
| 84  | MG   | B     | 1820 | 1/1   | 0.68 | 0.11 | 66,66,66,66                 | 0     |
| 84  | MG   | 1     | 3847 | 1/1   | 0.68 | 0.13 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3472 | 1/1   | 0.69 | 0.25 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3554 | 1/1   | 0.69 | 0.20 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3506 | 1/1   | 0.69 | 0.13 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3426 | 1/1   | 0.69 | 0.20 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3571 | 1/1   | 0.69 | 0.07 | 94,94,94,94                 | 0     |
| 84  | MG   | AS    | 3725 | 1/1   | 0.69 | 0.06 | 89,89,89,89                 | 0     |
| 84  | MG   | 1     | 3763 | 1/1   | 0.70 | 0.11 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3807 | 1/1   | 0.70 | 0.28 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3845 | 1/1   | 0.70 | 0.25 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3817 | 1/1   | 0.70 | 0.23 | 101,101,101,101             | 0     |
| 84  | MG   | CM    | 1805 | 1/1   | 0.70 | 0.33 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3856 | 1/1   | 0.70 | 0.24 | 91,91,91,91                 | 0     |
| 84  | MG   | 1     | 3609 | 1/1   | 0.70 | 0.13 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3570 | 1/1   | 0.70 | 0.18 | 87,87,87,87                 | 0     |
| 84  | MG   | 1     | 3624 | 1/1   | 0.70 | 0.09 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3606 | 1/1   | 0.70 | 0.32 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3667 | 1/1   | 0.70 | 0.07 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3717 | 1/1   | 0.70 | 0.25 | 54,54,54,54                 | 0     |
| 84  | MG   | Y     | 202  | 1/1   | 0.70 | 0.17 | 108,108,108,108             | 0     |
| 84  | MG   | 1     | 3830 | 1/1   | 0.70 | 0.14 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3428 | 1/1   | 0.70 | 0.18 | 71,71,71,71                 | 0     |
| 84  | MG   | AX    | 402  | 1/1   | 0.71 | 0.12 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3737 | 1/1   | 0.71 | 0.33 | 107,107,107,107             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | B     | 1835 | 1/1   | 0.71 | 0.13 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3741 | 1/1   | 0.71 | 0.16 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3548 | 1/1   | 0.71 | 0.24 | 48,48,48,48                 | 0     |
| 84  | MG   | AS    | 3749 | 1/1   | 0.71 | 0.24 | 73,73,73,73                 | 0     |
| 84  | MG   | 1     | 3591 | 1/1   | 0.71 | 0.10 | 45,45,45,45                 | 0     |
| 84  | MG   | B     | 1860 | 1/1   | 0.71 | 0.20 | 73,73,73,73                 | 0     |
| 84  | MG   | 1     | 3482 | 1/1   | 0.71 | 0.12 | 99,99,99,99                 | 0     |
| 84  | MG   | 1     | 3745 | 1/1   | 0.71 | 0.24 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3572 | 1/1   | 0.71 | 0.29 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3748 | 1/1   | 0.71 | 0.23 | 86,86,86,86                 | 0     |
| 84  | MG   | 1     | 3661 | 1/1   | 0.71 | 0.15 | 102,102,102,102             | 0     |
| 84  | MG   | 1     | 3412 | 1/1   | 0.71 | 0.15 | 66,66,66,66                 | 0     |
| 84  | MG   | B     | 1831 | 1/1   | 0.71 | 0.18 | 79,79,79,79                 | 0     |
| 84  | MG   | 1     | 3850 | 1/1   | 0.71 | 0.07 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3443 | 1/1   | 0.71 | 0.25 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3460 | 1/1   | 0.72 | 0.15 | 48,48,48,48                 | 0     |
| 84  | MG   | B     | 1868 | 1/1   | 0.72 | 0.15 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3461 | 1/1   | 0.72 | 0.26 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3692 | 1/1   | 0.72 | 0.20 | 56,56,56,56                 | 0     |
| 84  | MG   | B     | 1897 | 1/1   | 0.72 | 0.20 | 94,94,94,94                 | 0     |
| 84  | MG   | 1     | 3418 | 1/1   | 0.72 | 0.10 | 64,64,64,64                 | 0     |
| 84  | MG   | CM    | 1823 | 1/1   | 0.72 | 0.28 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3516 | 1/1   | 0.72 | 0.09 | 86,86,86,86                 | 0     |
| 84  | MG   | E     | 301  | 1/1   | 0.72 | 0.11 | 54,54,54,54                 | 0     |
| 84  | MG   | CM    | 1843 | 1/1   | 0.72 | 0.16 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3528 | 1/1   | 0.72 | 0.16 | 94,94,94,94                 | 0     |
| 84  | MG   | 1     | 3806 | 1/1   | 0.72 | 0.18 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3587 | 1/1   | 0.72 | 0.16 | 96,96,96,96                 | 0     |
| 84  | MG   | AS    | 3592 | 1/1   | 0.72 | 0.21 | 66,66,66,66                 | 0     |
| 84  | MG   | AD    | 201  | 1/1   | 0.72 | 0.26 | 58,58,58,58                 | 0     |
| 84  | MG   | 1     | 3813 | 1/1   | 0.72 | 0.08 | 69,69,69,69                 | 0     |
| 84  | MG   | AS    | 3615 | 1/1   | 0.72 | 0.12 | 102,102,102,102             | 0     |
| 84  | MG   | AS    | 3654 | 1/1   | 0.73 | 0.41 | 87,87,87,87                 | 0     |
| 84  | MG   | AS    | 3575 | 1/1   | 0.73 | 0.14 | 38,38,38,38                 | 0     |
| 84  | MG   | AS    | 3435 | 1/1   | 0.73 | 0.22 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3534 | 1/1   | 0.73 | 0.28 | 54,54,54,54                 | 0     |
| 84  | MG   | B     | 1806 | 1/1   | 0.73 | 0.23 | 99,99,99,99                 | 0     |
| 84  | MG   | 1     | 3530 | 1/1   | 0.73 | 0.10 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3709 | 1/1   | 0.73 | 0.10 | 53,53,53,53                 | 0     |
| 84  | MG   | AS    | 3484 | 1/1   | 0.73 | 0.16 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3745 | 1/1   | 0.73 | 0.13 | 104,104,104,104             | 0     |
| 84  | MG   | AS    | 3697 | 1/1   | 0.73 | 0.19 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | a     | 201  | 1/1   | 0.73 | 0.13 | 78,78,78,78                 | 0     |
| 84  | MG   | AS    | 3552 | 1/1   | 0.73 | 0.20 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3625 | 1/1   | 0.73 | 0.32 | 86,86,86,86                 | 0     |
| 84  | MG   | 1     | 3538 | 1/1   | 0.73 | 0.17 | 59,59,59,59                 | 0     |
| 84  | MG   | AS    | 3625 | 1/1   | 0.73 | 0.09 | 66,66,66,66                 | 0     |
| 84  | MG   | AS    | 3567 | 1/1   | 0.73 | 0.14 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3515 | 1/1   | 0.73 | 0.24 | 66,66,66,66                 | 0     |
| 84  | MG   | AS    | 3516 | 1/1   | 0.73 | 0.12 | 90,90,90,90                 | 0     |
| 84  | MG   | 1     | 3693 | 1/1   | 0.73 | 0.16 | 53,53,53,53                 | 0     |
| 84  | MG   | AS    | 3572 | 1/1   | 0.73 | 0.22 | 94,94,94,94                 | 0     |
| 84  | MG   | AS    | 3612 | 1/1   | 0.74 | 0.21 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3563 | 1/1   | 0.74 | 0.18 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3545 | 1/1   | 0.74 | 0.12 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3641 | 1/1   | 0.74 | 0.14 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3654 | 1/1   | 0.74 | 0.23 | 102,102,102,102             | 0     |
| 84  | MG   | 1     | 3411 | 1/1   | 0.74 | 0.15 | 90,90,90,90                 | 0     |
| 84  | MG   | AS    | 3757 | 1/1   | 0.74 | 0.23 | 65,65,65,65                 | 0     |
| 84  | MG   | B     | 1892 | 1/1   | 0.74 | 0.23 | 81,81,81,81                 | 0     |
| 84  | MG   | CM    | 1877 | 1/1   | 0.74 | 0.12 | 97,97,97,97                 | 0     |
| 84  | MG   | AS    | 3642 | 1/1   | 0.74 | 0.09 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3832 | 1/1   | 0.74 | 0.22 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3686 | 1/1   | 0.74 | 0.17 | 75,75,75,75                 | 0     |
| 84  | MG   | AS    | 3718 | 1/1   | 0.75 | 0.11 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3527 | 1/1   | 0.75 | 0.15 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3672 | 1/1   | 0.75 | 0.23 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3656 | 1/1   | 0.75 | 0.16 | 70,70,70,70                 | 0     |
| 84  | MG   | B     | 1804 | 1/1   | 0.75 | 0.15 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3704 | 1/1   | 0.75 | 0.17 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3752 | 1/1   | 0.75 | 0.20 | 77,77,77,77                 | 0     |
| 84  | MG   | B     | 1895 | 1/1   | 0.75 | 0.15 | 78,78,78,78                 | 0     |
| 84  | MG   | AS    | 3545 | 1/1   | 0.75 | 0.23 | 84,84,84,84                 | 0     |
| 84  | MG   | AS    | 3611 | 1/1   | 0.75 | 0.23 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3804 | 1/1   | 0.75 | 0.18 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3828 | 1/1   | 0.75 | 0.27 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3509 | 1/1   | 0.75 | 0.12 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3504 | 1/1   | 0.75 | 0.18 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3647 | 1/1   | 0.75 | 0.21 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3630 | 1/1   | 0.75 | 0.16 | 74,74,74,74                 | 0     |
| 84  | MG   | B     | 1845 | 1/1   | 0.75 | 0.13 | 89,89,89,89                 | 0     |
| 84  | MG   | y     | 201  | 1/1   | 0.75 | 0.11 | 63,63,63,63                 | 0     |
| 84  | MG   | B     | 1857 | 1/1   | 0.75 | 0.21 | 50,50,50,50                 | 0     |
| 84  | MG   | AS    | 3645 | 1/1   | 0.75 | 0.23 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3495 | 1/1   | 0.75 | 0.20 | 91,91,91,91                 | 0     |
| 84  | MG   | 1     | 3685 | 1/1   | 0.75 | 0.09 | 96,96,96,96                 | 0     |
| 84  | MG   | 1     | 3414 | 1/1   | 0.76 | 0.29 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3489 | 1/1   | 0.76 | 0.35 | 67,67,67,67                 | 0     |
| 84  | MG   | AZ    | 301  | 1/1   | 0.76 | 0.16 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3620 | 1/1   | 0.76 | 0.13 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3622 | 1/1   | 0.76 | 0.15 | 74,74,74,74                 | 0     |
| 84  | MG   | BZ    | 201  | 1/1   | 0.76 | 0.10 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3782 | 1/1   | 0.76 | 0.11 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3558 | 1/1   | 0.76 | 0.13 | 69,69,69,69                 | 0     |
| 84  | MG   | 0     | 201  | 1/1   | 0.76 | 0.13 | 87,87,87,87                 | 0     |
| 84  | MG   | B     | 1844 | 1/1   | 0.76 | 0.12 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3758 | 1/1   | 0.76 | 0.17 | 67,67,67,67                 | 0     |
| 84  | MG   | 1     | 3683 | 1/1   | 0.76 | 0.19 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3559 | 1/1   | 0.76 | 0.09 | 23,23,23,23                 | 0     |
| 84  | MG   | CM    | 1841 | 1/1   | 0.76 | 0.09 | 42,42,42,42                 | 0     |
| 84  | MG   | 1     | 3749 | 1/1   | 0.76 | 0.16 | 77,77,77,77                 | 0     |
| 84  | MG   | CM    | 1844 | 1/1   | 0.76 | 0.20 | 78,78,78,78                 | 0     |
| 84  | MG   | CM    | 1845 | 1/1   | 0.76 | 0.12 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3596 | 1/1   | 0.76 | 0.11 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3412 | 1/1   | 0.76 | 0.25 | 84,84,84,84                 | 0     |
| 84  | MG   | AS    | 3602 | 1/1   | 0.76 | 0.17 | 76,76,76,76                 | 0     |
| 84  | MG   | CM    | 1857 | 1/1   | 0.76 | 0.10 | 83,83,83,83                 | 0     |
| 84  | MG   | CM    | 1869 | 1/1   | 0.76 | 0.25 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3674 | 1/1   | 0.76 | 0.17 | 67,67,67,67                 | 0     |
| 84  | MG   | B     | 1809 | 1/1   | 0.76 | 0.19 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3665 | 1/1   | 0.76 | 0.12 | 75,75,75,75                 | 0     |
| 84  | MG   | AS    | 3724 | 1/1   | 0.76 | 0.12 | 87,87,87,87                 | 0     |
| 84  | MG   | B     | 1872 | 1/1   | 0.76 | 0.20 | 95,95,95,95                 | 0     |
| 84  | MG   | 1     | 3614 | 1/1   | 0.77 | 0.13 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3631 | 1/1   | 0.77 | 0.22 | 53,53,53,53                 | 0     |
| 84  | MG   | B     | 1855 | 1/1   | 0.77 | 0.14 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3634 | 1/1   | 0.77 | 0.17 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3635 | 1/1   | 0.77 | 0.23 | 76,76,76,76                 | 0     |
| 84  | MG   | AY    | 401  | 1/1   | 0.77 | 0.20 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3638 | 1/1   | 0.77 | 0.16 | 76,76,76,76                 | 0     |
| 84  | MG   | B     | 1856 | 1/1   | 0.77 | 0.15 | 148,148,148,148             | 0     |
| 84  | MG   | 1     | 3568 | 1/1   | 0.77 | 0.26 | 67,67,67,67                 | 0     |
| 84  | MG   | 1     | 3579 | 1/1   | 0.77 | 0.23 | 93,93,93,93                 | 0     |
| 84  | MG   | 1     | 3630 | 1/1   | 0.77 | 0.10 | 39,39,39,39                 | 0     |
| 84  | MG   | B     | 1812 | 1/1   | 0.77 | 0.19 | 52,52,52,52                 | 0     |
| 84  | MG   | 1     | 3789 | 1/1   | 0.77 | 0.09 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3530 | 1/1   | 0.77 | 0.26 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3437 | 1/1   | 0.77 | 0.17 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3535 | 1/1   | 0.77 | 0.40 | 111,111,111,111             | 0     |
| 84  | MG   | 1     | 3700 | 1/1   | 0.77 | 0.22 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3446 | 1/1   | 0.77 | 0.12 | 55,55,55,55                 | 0     |
| 84  | MG   | CM    | 1838 | 1/1   | 0.77 | 0.19 | 101,101,101,101             | 0     |
| 84  | MG   | 1     | 3765 | 1/1   | 0.77 | 0.25 | 98,98,98,98                 | 0     |
| 84  | MG   | 1     | 3703 | 1/1   | 0.77 | 0.17 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3670 | 1/1   | 0.77 | 0.20 | 77,77,77,77                 | 0     |
| 84  | MG   | B     | 1841 | 1/1   | 0.77 | 0.34 | 73,73,73,73                 | 0     |
| 84  | MG   | AS    | 3681 | 1/1   | 0.77 | 0.23 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3682 | 1/1   | 0.77 | 0.24 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3485 | 1/1   | 0.77 | 0.14 | 91,91,91,91                 | 0     |
| 84  | MG   | B     | 1899 | 1/1   | 0.77 | 0.11 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3695 | 1/1   | 0.77 | 0.14 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3758 | 1/1   | 0.77 | 0.23 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3582 | 1/1   | 0.77 | 0.16 | 49,49,49,49                 | 0     |
| 84  | MG   | 1     | 3536 | 1/1   | 0.77 | 0.26 | 73,73,73,73                 | 0     |
| 84  | MG   | AS    | 3704 | 1/1   | 0.77 | 0.11 | 75,75,75,75                 | 0     |
| 84  | MG   | AS    | 3776 | 1/1   | 0.77 | 0.17 | 88,88,88,88                 | 0     |
| 84  | MG   | 1     | 3803 | 1/1   | 0.78 | 0.09 | 63,63,63,63                 | 0     |
| 84  | MG   | AS    | 3556 | 1/1   | 0.78 | 0.09 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3827 | 1/1   | 0.78 | 0.22 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3687 | 1/1   | 0.78 | 0.12 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3583 | 1/1   | 0.78 | 0.10 | 81,81,81,81                 | 0     |
| 84  | MG   | 1     | 3610 | 1/1   | 0.78 | 0.14 | 67,67,67,67                 | 0     |
| 84  | MG   | 1     | 3809 | 1/1   | 0.78 | 0.11 | 179,179,179,179             | 0     |
| 84  | MG   | CM    | 1831 | 1/1   | 0.78 | 0.25 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3670 | 1/1   | 0.78 | 0.14 | 98,98,98,98                 | 0     |
| 84  | MG   | AS    | 3528 | 1/1   | 0.78 | 0.20 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3553 | 1/1   | 0.78 | 0.08 | 66,66,66,66                 | 0     |
| 84  | MG   | 1     | 3791 | 1/1   | 0.78 | 0.09 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3820 | 1/1   | 0.78 | 0.34 | 88,88,88,88                 | 0     |
| 84  | MG   | AS    | 3534 | 1/1   | 0.78 | 0.15 | 113,113,113,113             | 0     |
| 84  | MG   | 1     | 3578 | 1/1   | 0.78 | 0.30 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3779 | 1/1   | 0.78 | 0.11 | 60,60,60,60                 | 0     |
| 84  | MG   | B     | 1814 | 1/1   | 0.78 | 0.26 | 40,40,40,40                 | 0     |
| 84  | MG   | AS    | 3406 | 1/1   | 0.78 | 0.12 | 122,122,122,122             | 0     |
| 84  | MG   | B     | 1818 | 1/1   | 0.78 | 0.20 | 57,57,57,57                 | 0     |
| 84  | MG   | BB    | 302  | 1/1   | 0.78 | 0.19 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3547 | 1/1   | 0.78 | 0.13 | 98,98,98,98                 | 0     |
| 84  | MG   | AS    | 3748 | 1/1   | 0.78 | 0.15 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3694 | 1/1   | 0.78 | 0.13 | 84,84,84,84                 | 0     |
| 85  | ZN   | d     | 101  | 1/1   | 0.78 | 0.09 | 314,314,314,314             | 0     |
| 84  | MG   | B     | 1861 | 1/1   | 0.79 | 0.21 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3696 | 1/1   | 0.79 | 0.27 | 78,78,78,78                 | 0     |
| 84  | MG   | B     | 1807 | 1/1   | 0.79 | 0.26 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3468 | 1/1   | 0.79 | 0.13 | 40,40,40,40                 | 0     |
| 84  | MG   | AT    | 203  | 1/1   | 0.79 | 0.18 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3623 | 1/1   | 0.79 | 0.12 | 70,70,70,70                 | 0     |
| 84  | MG   | B     | 1884 | 1/1   | 0.79 | 0.18 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3707 | 1/1   | 0.79 | 0.17 | 42,42,42,42                 | 0     |
| 84  | MG   | 1     | 3573 | 1/1   | 0.79 | 0.14 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3575 | 1/1   | 0.79 | 0.11 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3496 | 1/1   | 0.79 | 0.29 | 69,69,69,69                 | 0     |
| 84  | MG   | AS    | 3504 | 1/1   | 0.79 | 0.10 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3505 | 1/1   | 0.79 | 0.12 | 90,90,90,90                 | 0     |
| 84  | MG   | 1     | 3533 | 1/1   | 0.79 | 0.25 | 37,37,37,37                 | 0     |
| 84  | MG   | 1     | 3771 | 1/1   | 0.79 | 0.17 | 64,64,64,64                 | 0     |
| 84  | MG   | B     | 1828 | 1/1   | 0.79 | 0.18 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3431 | 1/1   | 0.79 | 0.23 | 41,41,41,41                 | 0     |
| 84  | MG   | B     | 1832 | 1/1   | 0.79 | 0.12 | 92,92,92,92                 | 0     |
| 84  | MG   | 1     | 3485 | 1/1   | 0.79 | 0.09 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3427 | 1/1   | 0.79 | 0.20 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3519 | 1/1   | 0.79 | 0.16 | 110,110,110,110             | 0     |
| 84  | MG   | AS    | 3655 | 1/1   | 0.79 | 0.21 | 99,99,99,99                 | 0     |
| 84  | MG   | o     | 301  | 1/1   | 0.79 | 0.30 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3658 | 1/1   | 0.79 | 0.21 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3478 | 1/1   | 0.79 | 0.18 | 53,53,53,53                 | 0     |
| 84  | MG   | 1     | 3514 | 1/1   | 0.79 | 0.22 | 87,87,87,87                 | 0     |
| 84  | MG   | 1     | 3637 | 1/1   | 0.79 | 0.21 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3639 | 1/1   | 0.79 | 0.11 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3480 | 1/1   | 0.79 | 0.10 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3606 | 1/1   | 0.79 | 0.20 | 83,83,83,83                 | 0     |
| 84  | MG   | CM    | 1856 | 1/1   | 0.79 | 0.21 | 88,88,88,88                 | 0     |
| 84  | MG   | 1     | 3592 | 1/1   | 0.79 | 0.17 | 73,73,73,73                 | 0     |
| 84  | MG   | CM    | 1868 | 1/1   | 0.79 | 0.25 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3519 | 1/1   | 0.79 | 0.26 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3613 | 1/1   | 0.79 | 0.23 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3439 | 1/1   | 0.79 | 0.27 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3683 | 1/1   | 0.79 | 0.19 | 61,61,61,61                 | 0     |
| 84  | MG   | AS    | 3684 | 1/1   | 0.79 | 0.19 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3795 | 1/1   | 0.79 | 0.09 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3616 | 1/1   | 0.79 | 0.21 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | v     | 302  | 1/1   | 0.80 | 0.14 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3769 | 1/1   | 0.80 | 0.12 | 51,51,51,51                 | 0     |
| 84  | MG   | AS    | 3422 | 1/1   | 0.80 | 0.45 | 36,36,36,36                 | 0     |
| 84  | MG   | B     | 1846 | 1/1   | 0.80 | 0.18 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3580 | 1/1   | 0.80 | 0.27 | 60,60,60,60                 | 0     |
| 84  | MG   | AB    | 201  | 1/1   | 0.80 | 0.10 | 55,55,55,55                 | 0     |
| 84  | MG   | AS    | 3786 | 1/1   | 0.80 | 0.09 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3562 | 1/1   | 0.80 | 0.07 | 66,66,66,66                 | 0     |
| 84  | MG   | 1     | 3598 | 1/1   | 0.80 | 0.25 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3802 | 1/1   | 0.80 | 0.13 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3699 | 1/1   | 0.80 | 0.24 | 79,79,79,79                 | 0     |
| 84  | MG   | AS    | 3700 | 1/1   | 0.80 | 0.17 | 95,95,95,95                 | 0     |
| 84  | MG   | 1     | 3669 | 1/1   | 0.80 | 0.19 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3497 | 1/1   | 0.80 | 0.33 | 78,78,78,78                 | 0     |
| 84  | MG   | B     | 1862 | 1/1   | 0.80 | 0.21 | 76,76,76,76                 | 0     |
| 84  | MG   | BB    | 301  | 1/1   | 0.80 | 0.22 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3555 | 1/1   | 0.80 | 0.10 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3708 | 1/1   | 0.80 | 0.10 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3603 | 1/1   | 0.80 | 0.24 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3783 | 1/1   | 0.80 | 0.09 | 66,66,66,66                 | 0     |
| 84  | MG   | CB    | 202  | 1/1   | 0.80 | 0.12 | 65,65,65,65                 | 0     |
| 84  | MG   | AS    | 3712 | 1/1   | 0.80 | 0.11 | 94,94,94,94                 | 0     |
| 84  | MG   | 1     | 3515 | 1/1   | 0.80 | 0.17 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3564 | 1/1   | 0.80 | 0.11 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3849 | 1/1   | 0.80 | 0.09 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3810 | 1/1   | 0.80 | 0.17 | 144,144,144,144             | 0     |
| 84  | MG   | 1     | 3853 | 1/1   | 0.80 | 0.09 | 106,106,106,106             | 0     |
| 84  | MG   | B     | 1893 | 1/1   | 0.80 | 0.18 | 87,87,87,87                 | 0     |
| 84  | MG   | AS    | 3646 | 1/1   | 0.80 | 0.23 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3571 | 1/1   | 0.80 | 0.15 | 84,84,84,84                 | 0     |
| 84  | MG   | 1     | 3762 | 1/1   | 0.80 | 0.19 | 82,82,82,82                 | 0     |
| 84  | MG   | B     | 1896 | 1/1   | 0.80 | 0.10 | 78,78,78,78                 | 0     |
| 84  | MG   | B     | 1826 | 1/1   | 0.80 | 0.11 | 76,76,76,76                 | 0     |
| 84  | MG   | AS    | 3731 | 1/1   | 0.80 | 0.22 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3499 | 1/1   | 0.80 | 0.36 | 50,50,50,50                 | 0     |
| 84  | MG   | AS    | 3583 | 1/1   | 0.80 | 0.34 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3466 | 1/1   | 0.80 | 0.12 | 79,79,79,79                 | 0     |
| 84  | MG   | AS    | 3659 | 1/1   | 0.80 | 0.15 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3790 | 1/1   | 0.80 | 0.18 | 56,56,56,56                 | 0     |
| 84  | MG   | AS    | 3586 | 1/1   | 0.80 | 0.24 | 61,61,61,61                 | 0     |
| 84  | MG   | o     | 303  | 1/1   | 0.80 | 0.28 | 56,56,56,56                 | 0     |
| 84  | MG   | AS    | 3666 | 1/1   | 0.80 | 0.12 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | R     | 201  | 1/1   | 0.80 | 0.28 | 61,61,61,61                 | 0     |
| 84  | MG   | Y     | 201  | 1/1   | 0.80 | 0.22 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3527 | 1/1   | 0.80 | 0.14 | 75,75,75,75                 | 0     |
| 84  | MG   | v     | 301  | 1/1   | 0.80 | 0.15 | 56,56,56,56                 | 0     |
| 84  | MG   | AS    | 3603 | 1/1   | 0.80 | 0.23 | 38,38,38,38                 | 0     |
| 84  | MG   | AS    | 3610 | 1/1   | 0.81 | 0.14 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3457 | 1/1   | 0.81 | 0.24 | 43,43,43,43                 | 0     |
| 84  | MG   | AS    | 3770 | 1/1   | 0.81 | 0.08 | 61,61,61,61                 | 0     |
| 84  | MG   | AS    | 3691 | 1/1   | 0.81 | 0.09 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3638 | 1/1   | 0.81 | 0.15 | 89,89,89,89                 | 0     |
| 84  | MG   | AS    | 3408 | 1/1   | 0.81 | 0.10 | 87,87,87,87                 | 0     |
| 84  | MG   | AS    | 3788 | 1/1   | 0.81 | 0.11 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3402 | 1/1   | 0.81 | 0.29 | 69,69,69,69                 | 0     |
| 84  | MG   | AS    | 3420 | 1/1   | 0.81 | 0.15 | 50,50,50,50                 | 0     |
| 84  | MG   | AT    | 201  | 1/1   | 0.81 | 0.12 | 59,59,59,59                 | 0     |
| 84  | MG   | B     | 1858 | 1/1   | 0.81 | 0.12 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3542 | 1/1   | 0.81 | 0.26 | 55,55,55,55                 | 0     |
| 84  | MG   | 1     | 3646 | 1/1   | 0.81 | 0.17 | 86,86,86,86                 | 0     |
| 84  | MG   | AS    | 3621 | 1/1   | 0.81 | 0.07 | 61,61,61,61                 | 0     |
| 84  | MG   | B     | 1810 | 1/1   | 0.81 | 0.22 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3684 | 1/1   | 0.81 | 0.11 | 86,86,86,86                 | 0     |
| 84  | MG   | B     | 1867 | 1/1   | 0.81 | 0.18 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3863 | 1/1   | 0.81 | 0.20 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3440 | 1/1   | 0.81 | 0.22 | 42,42,42,42                 | 0     |
| 84  | MG   | BL    | 201  | 1/1   | 0.81 | 0.15 | 66,66,66,66                 | 0     |
| 84  | MG   | 1     | 3463 | 1/1   | 0.81 | 0.26 | 32,32,32,32                 | 0     |
| 84  | MG   | B     | 1878 | 1/1   | 0.81 | 0.19 | 102,102,102,102             | 0     |
| 84  | MG   | 1     | 3650 | 1/1   | 0.81 | 0.23 | 59,59,59,59                 | 0     |
| 84  | MG   | j     | 301  | 1/1   | 0.81 | 0.14 | 65,65,65,65                 | 0     |
| 84  | MG   | AS    | 3475 | 1/1   | 0.81 | 0.10 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3478 | 1/1   | 0.81 | 0.09 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3651 | 1/1   | 0.81 | 0.25 | 55,55,55,55                 | 0     |
| 84  | MG   | 1     | 3560 | 1/1   | 0.81 | 0.09 | 66,66,66,66                 | 0     |
| 84  | MG   | B     | 1829 | 1/1   | 0.81 | 0.15 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3544 | 1/1   | 0.81 | 0.10 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3491 | 1/1   | 0.81 | 0.07 | 39,39,39,39                 | 0     |
| 84  | MG   | CM    | 1832 | 1/1   | 0.81 | 0.19 | 99,99,99,99                 | 0     |
| 84  | MG   | AS    | 3498 | 1/1   | 0.81 | 0.21 | 48,48,48,48                 | 0     |
| 84  | MG   | AS    | 3500 | 1/1   | 0.81 | 0.20 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3503 | 1/1   | 0.81 | 0.15 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3579 | 1/1   | 0.81 | 0.18 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3793 | 1/1   | 0.81 | 0.08 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3740 | 1/1   | 0.81 | 0.10 | 40,40,40,40                 | 0     |
| 84  | MG   | 1     | 3444 | 1/1   | 0.81 | 0.22 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3737 | 1/1   | 0.81 | 0.15 | 57,57,57,57                 | 0     |
| 84  | MG   | B     | 1839 | 1/1   | 0.81 | 0.08 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3618 | 1/1   | 0.81 | 0.19 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3426 | 1/1   | 0.81 | 0.27 | 51,51,51,51                 | 0     |
| 84  | MG   | G     | 301  | 1/1   | 0.81 | 0.10 | 68,68,68,68                 | 0     |
| 84  | MG   | AC    | 101  | 1/1   | 0.81 | 0.07 | 59,59,59,59                 | 0     |
| 84  | MG   | R     | 204  | 1/1   | 0.81 | 0.23 | 55,55,55,55                 | 0     |
| 84  | MG   | 1     | 3597 | 1/1   | 0.81 | 0.21 | 97,97,97,97                 | 1     |
| 84  | MG   | CM    | 1879 | 1/1   | 0.81 | 0.15 | 61,61,61,61                 | 0     |
| 84  | MG   | DA    | 201  | 1/1   | 0.81 | 0.17 | 86,86,86,86                 | 0     |
| 84  | MG   | 1     | 3493 | 1/1   | 0.81 | 0.23 | 65,65,65,65                 | 0     |
| 84  | MG   | AS    | 3526 | 1/1   | 0.81 | 0.17 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3609 | 1/1   | 0.81 | 0.19 | 98,98,98,98                 | 0     |
| 84  | MG   | AS    | 3719 | 1/1   | 0.82 | 0.17 | 95,95,95,95                 | 0     |
| 84  | MG   | AS    | 3688 | 1/1   | 0.82 | 0.06 | 120,120,120,120             | 0     |
| 84  | MG   | 1     | 3555 | 1/1   | 0.82 | 0.25 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3780 | 1/1   | 0.82 | 0.07 | 35,35,35,35                 | 0     |
| 84  | MG   | 1     | 3846 | 1/1   | 0.82 | 0.16 | 99,99,99,99                 | 0     |
| 84  | MG   | AS    | 3784 | 1/1   | 0.82 | 0.07 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3451 | 1/1   | 0.82 | 0.23 | 72,72,72,72                 | 0     |
| 84  | MG   | CM    | 1836 | 1/1   | 0.82 | 0.14 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3787 | 1/1   | 0.82 | 0.16 | 96,96,96,96                 | 0     |
| 84  | MG   | 1     | 3406 | 1/1   | 0.82 | 0.17 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3563 | 1/1   | 0.82 | 0.23 | 129,129,129,129             | 0     |
| 84  | MG   | 1     | 3735 | 1/1   | 0.82 | 0.10 | 87,87,87,87                 | 0     |
| 84  | MG   | 1     | 3640 | 1/1   | 0.82 | 0.16 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3725 | 1/1   | 0.82 | 0.16 | 90,90,90,90                 | 0     |
| 84  | MG   | AS    | 3587 | 1/1   | 0.82 | 0.17 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3524 | 1/1   | 0.82 | 0.11 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3859 | 1/1   | 0.82 | 0.24 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3767 | 1/1   | 0.82 | 0.07 | 58,58,58,58                 | 0     |
| 84  | MG   | CM    | 1861 | 1/1   | 0.82 | 0.09 | 92,92,92,92                 | 0     |
| 84  | MG   | AS    | 3599 | 1/1   | 0.82 | 0.11 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3869 | 1/1   | 0.82 | 0.12 | 95,95,95,95                 | 0     |
| 84  | MG   | AS    | 3711 | 1/1   | 0.82 | 0.20 | 78,78,78,78                 | 0     |
| 84  | MG   | AS    | 3431 | 1/1   | 0.82 | 0.14 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3796 | 1/1   | 0.82 | 0.10 | 105,105,105,105             | 0     |
| 84  | MG   | 1     | 3835 | 1/1   | 0.82 | 0.13 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3425 | 1/1   | 0.82 | 0.29 | 36,36,36,36                 | 0     |
| 84  | MG   | 1     | 3642 | 1/1   | 0.82 | 0.09 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3842 | 1/1   | 0.82 | 0.13 | 88,88,88,88                 | 0     |
| 84  | MG   | AS    | 3573 | 1/1   | 0.82 | 0.17 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3597 | 1/1   | 0.83 | 0.15 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3644 | 1/1   | 0.83 | 0.12 | 62,62,62,62                 | 0     |
| 84  | MG   | R     | 202  | 1/1   | 0.83 | 0.16 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3707 | 1/1   | 0.83 | 0.17 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3562 | 1/1   | 0.83 | 0.24 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3680 | 1/1   | 0.83 | 0.20 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3607 | 1/1   | 0.83 | 0.23 | 56,56,56,56                 | 0     |
| 84  | MG   | CM    | 1821 | 1/1   | 0.83 | 0.30 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3453 | 1/1   | 0.83 | 0.08 | 54,54,54,54                 | 0     |
| 84  | MG   | CM    | 1825 | 1/1   | 0.83 | 0.21 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3581 | 1/1   | 0.83 | 0.16 | 70,70,70,70                 | 0     |
| 84  | MG   | o     | 302  | 1/1   | 0.83 | 0.14 | 46,46,46,46                 | 0     |
| 84  | MG   | AS    | 3403 | 1/1   | 0.83 | 0.07 | 84,84,84,84                 | 0     |
| 84  | MG   | 1     | 3714 | 1/1   | 0.83 | 0.13 | 77,77,77,77                 | 0     |
| 84  | MG   | CM    | 1834 | 1/1   | 0.83 | 0.22 | 130,130,130,130             | 0     |
| 84  | MG   | B     | 1811 | 1/1   | 0.83 | 0.16 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3410 | 1/1   | 0.83 | 0.37 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3458 | 1/1   | 0.83 | 0.21 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3805 | 1/1   | 0.83 | 0.10 | 84,84,84,84                 | 0     |
| 84  | MG   | 1     | 3753 | 1/1   | 0.83 | 0.42 | 79,79,79,79                 | 0     |
| 84  | MG   | AS    | 3423 | 1/1   | 0.83 | 0.21 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3552 | 1/1   | 0.83 | 0.14 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3677 | 1/1   | 0.83 | 0.21 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3581 | 1/1   | 0.83 | 0.17 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3584 | 1/1   | 0.83 | 0.17 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3627 | 1/1   | 0.83 | 0.29 | 72,72,72,72                 | 0     |
| 84  | MG   | B     | 1823 | 1/1   | 0.83 | 0.20 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3726 | 1/1   | 0.83 | 0.13 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3860 | 1/1   | 0.83 | 0.12 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3685 | 1/1   | 0.83 | 0.23 | 67,67,67,67                 | 0     |
| 84  | MG   | CM    | 1876 | 1/1   | 0.83 | 0.05 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3449 | 1/1   | 0.83 | 0.34 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3551 | 1/1   | 0.83 | 0.10 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3738 | 1/1   | 0.83 | 0.23 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3865 | 1/1   | 0.83 | 0.15 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3553 | 1/1   | 0.83 | 0.11 | 96,96,96,96                 | 0     |
| 84  | MG   | 1     | 3586 | 1/1   | 0.83 | 0.26 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3743 | 1/1   | 0.83 | 0.21 | 73,73,73,73                 | 0     |
| 84  | MG   | AS    | 3742 | 1/1   | 0.84 | 0.22 | 93,93,93,93                 | 0     |
| 84  | MG   | 1     | 3750 | 1/1   | 0.84 | 0.09 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3858 | 1/1   | 0.84 | 0.08 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3507 | 1/1   | 0.84 | 0.12 | 80,80,80,80                 | 0     |
| 84  | MG   | AS    | 3508 | 1/1   | 0.84 | 0.15 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3797 | 1/1   | 0.84 | 0.13 | 48,48,48,48                 | 0     |
| 84  | MG   | AS    | 3648 | 1/1   | 0.84 | 0.16 | 55,55,55,55                 | 0     |
| 84  | MG   | AS    | 3441 | 1/1   | 0.84 | 0.18 | 39,39,39,39                 | 0     |
| 84  | MG   | 1     | 3628 | 1/1   | 0.84 | 0.12 | 99,99,99,99                 | 0     |
| 84  | MG   | B     | 1888 | 1/1   | 0.84 | 0.10 | 59,59,59,59                 | 0     |
| 84  | MG   | AS    | 3653 | 1/1   | 0.84 | 0.15 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3839 | 1/1   | 0.84 | 0.32 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3517 | 1/1   | 0.84 | 0.10 | 50,50,50,50                 | 0     |
| 84  | MG   | AS    | 3458 | 1/1   | 0.84 | 0.11 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3673 | 1/1   | 0.84 | 0.29 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3767 | 1/1   | 0.84 | 0.17 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3520 | 1/1   | 0.84 | 0.15 | 66,66,66,66                 | 0     |
| 84  | MG   | AS    | 3523 | 1/1   | 0.84 | 0.13 | 103,103,103,103             | 0     |
| 84  | MG   | 1     | 3636 | 1/1   | 0.84 | 0.19 | 43,43,43,43                 | 0     |
| 84  | MG   | AS    | 3474 | 1/1   | 0.84 | 0.10 | 72,72,72,72                 | 0     |
| 84  | MG   | AS    | 3413 | 1/1   | 0.84 | 0.36 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3785 | 1/1   | 0.84 | 0.14 | 59,59,59,59                 | 0     |
| 84  | MG   | 3     | 201  | 1/1   | 0.84 | 0.22 | 63,63,63,63                 | 0     |
| 84  | MG   | AS    | 3668 | 1/1   | 0.84 | 0.17 | 68,68,68,68                 | 0     |
| 84  | MG   | 1     | 3659 | 1/1   | 0.84 | 0.11 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3454 | 1/1   | 0.84 | 0.25 | 59,59,59,59                 | 0     |
| 84  | MG   | k     | 401  | 1/1   | 0.84 | 0.09 | 71,71,71,71                 | 0     |
| 84  | MG   | CM    | 1862 | 1/1   | 0.84 | 0.07 | 66,66,66,66                 | 0     |
| 84  | MG   | AS    | 3577 | 1/1   | 0.84 | 0.11 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3434 | 1/1   | 0.84 | 0.45 | 47,47,47,47                 | 0     |
| 84  | MG   | AS    | 3680 | 1/1   | 0.84 | 0.06 | 108,108,108,108             | 0     |
| 84  | MG   | CM    | 1875 | 1/1   | 0.84 | 0.07 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3429 | 1/1   | 0.84 | 0.22 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3497 | 1/1   | 0.84 | 0.14 | 51,51,51,51                 | 0     |
| 84  | MG   | AS    | 3628 | 1/1   | 0.84 | 0.17 | 67,67,67,67                 | 0     |
| 84  | MG   | 1     | 3511 | 1/1   | 0.84 | 0.26 | 38,38,38,38                 | 0     |
| 84  | MG   | B     | 1838 | 1/1   | 0.84 | 0.18 | 38,38,38,38                 | 0     |
| 84  | MG   | 1     | 3648 | 1/1   | 0.84 | 0.09 | 63,63,63,63                 | 0     |
| 84  | MG   | AS    | 3543 | 1/1   | 0.84 | 0.12 | 66,66,66,66                 | 0     |
| 84  | MG   | AS    | 3544 | 1/1   | 0.84 | 0.25 | 52,52,52,52                 | 0     |
| 85  | ZN   | CB    | 201  | 1/1   | 0.84 | 0.06 | 296,296,296,296             | 0     |
| 84  | MG   | AS    | 3411 | 1/1   | 0.85 | 0.18 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3617 | 1/1   | 0.85 | 0.20 | 33,33,33,33                 | 0     |
| 84  | MG   | AS    | 3538 | 1/1   | 0.85 | 0.14 | 98,98,98,98                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | CA    | 201  | 1/1   | 0.85 | 0.11 | 58,58,58,58                 | 0     |
| 84  | MG   | 1     | 3677 | 1/1   | 0.85 | 0.12 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3496 | 1/1   | 0.85 | 0.20 | 52,52,52,52                 | 0     |
| 84  | MG   | B     | 1880 | 1/1   | 0.85 | 0.11 | 88,88,88,88                 | 0     |
| 84  | MG   | AS    | 3591 | 1/1   | 0.85 | 0.26 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3746 | 1/1   | 0.85 | 0.23 | 79,79,79,79                 | 0     |
| 84  | MG   | AS    | 3643 | 1/1   | 0.85 | 0.10 | 47,47,47,47                 | 0     |
| 84  | MG   | 1     | 3743 | 1/1   | 0.85 | 0.09 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3698 | 1/1   | 0.85 | 0.13 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3814 | 1/1   | 0.85 | 0.25 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3764 | 1/1   | 0.85 | 0.30 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3818 | 1/1   | 0.85 | 0.30 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3494 | 1/1   | 0.85 | 0.18 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3623 | 1/1   | 0.85 | 0.13 | 66,66,66,66                 | 0     |
| 84  | MG   | AB    | 202  | 1/1   | 0.85 | 0.11 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3602 | 1/1   | 0.85 | 0.09 | 57,57,57,57                 | 0     |
| 84  | MG   | 1     | 3699 | 1/1   | 0.85 | 0.13 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3500 | 1/1   | 0.85 | 0.44 | 58,58,58,58                 | 0     |
| 84  | MG   | 1     | 3702 | 1/1   | 0.85 | 0.11 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3864 | 1/1   | 0.85 | 0.06 | 46,46,46,46                 | 0     |
| 84  | MG   | AS    | 3660 | 1/1   | 0.85 | 0.11 | 95,95,95,95                 | 0     |
| 84  | MG   | 1     | 3550 | 1/1   | 0.85 | 0.32 | 56,56,56,56                 | 0     |
| 84  | MG   | B     | 1854 | 1/1   | 0.85 | 0.17 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3867 | 1/1   | 0.85 | 0.10 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3594 | 1/1   | 0.85 | 0.07 | 76,76,76,76                 | 0     |
| 84  | MG   | AS    | 3454 | 1/1   | 0.85 | 0.13 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3734 | 1/1   | 0.85 | 0.09 | 73,73,73,73                 | 0     |
| 84  | MG   | 1     | 3834 | 1/1   | 0.85 | 0.14 | 90,90,90,90                 | 0     |
| 84  | MG   | 1     | 3529 | 1/1   | 0.85 | 0.27 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3722 | 1/1   | 0.85 | 0.07 | 90,90,90,90                 | 0     |
| 84  | MG   | CM    | 1873 | 1/1   | 0.85 | 0.15 | 81,81,81,81                 | 0     |
| 84  | MG   | CM    | 1874 | 1/1   | 0.85 | 0.10 | 68,68,68,68                 | 0     |
| 84  | MG   | 1     | 3755 | 1/1   | 0.85 | 0.10 | 55,55,55,55                 | 0     |
| 84  | MG   | AT    | 204  | 1/1   | 0.85 | 0.23 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3676 | 1/1   | 0.85 | 0.11 | 61,61,61,61                 | 0     |
| 84  | MG   | B     | 1815 | 1/1   | 0.85 | 0.08 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3477 | 1/1   | 0.85 | 0.09 | 50,50,50,50                 | 0     |
| 84  | MG   | CW    | 201  | 1/1   | 0.85 | 0.16 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3626 | 1/1   | 0.85 | 0.23 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3734 | 1/1   | 0.85 | 0.15 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3523 | 1/1   | 0.85 | 0.14 | 84,84,84,84                 | 0     |
| 85  | ZN   | AH    | 201  | 1/1   | 0.85 | 0.08 | 232,232,232,232             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | k     | 402  | 1/1   | 0.85 | 0.27 | 98,98,98,98                 | 0     |
| 84  | MG   | 1     | 3532 | 1/1   | 0.85 | 0.17 | 44,44,44,44                 | 0     |
| 84  | MG   | B     | 1891 | 1/1   | 0.86 | 0.14 | 86,86,86,86                 | 0     |
| 84  | MG   | 1     | 3819 | 1/1   | 0.86 | 0.17 | 84,84,84,84                 | 0     |
| 84  | MG   | 1     | 3474 | 1/1   | 0.86 | 0.10 | 58,58,58,58                 | 0     |
| 84  | MG   | CM    | 1829 | 1/1   | 0.86 | 0.10 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3469 | 1/1   | 0.86 | 0.12 | 42,42,42,42                 | 0     |
| 84  | MG   | 1     | 3403 | 1/1   | 0.86 | 0.27 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3604 | 1/1   | 0.86 | 0.08 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3558 | 1/1   | 0.86 | 0.11 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3421 | 1/1   | 0.86 | 0.25 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3521 | 1/1   | 0.86 | 0.18 | 54,54,54,54                 | 0     |
| 84  | MG   | CM    | 1840 | 1/1   | 0.86 | 0.11 | 60,60,60,60                 | 0     |
| 84  | MG   | AP    | 203  | 1/1   | 0.86 | 0.16 | 86,86,86,86                 | 0     |
| 84  | MG   | B     | 1898 | 1/1   | 0.86 | 0.10 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3608 | 1/1   | 0.86 | 0.24 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3455 | 1/1   | 0.86 | 0.20 | 45,45,45,45                 | 0     |
| 84  | MG   | AS    | 3693 | 1/1   | 0.86 | 0.17 | 63,63,63,63                 | 0     |
| 84  | MG   | AT    | 202  | 1/1   | 0.86 | 0.06 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3537 | 1/1   | 0.86 | 0.16 | 27,27,27,27                 | 0     |
| 84  | MG   | 1     | 3607 | 1/1   | 0.86 | 0.20 | 72,72,72,72                 | 0     |
| 84  | MG   | AS    | 3486 | 1/1   | 0.86 | 0.21 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3705 | 1/1   | 0.86 | 0.14 | 68,68,68,68                 | 0     |
| 84  | MG   | AX    | 403  | 1/1   | 0.86 | 0.27 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3479 | 1/1   | 0.86 | 0.32 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3657 | 1/1   | 0.86 | 0.14 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3541 | 1/1   | 0.86 | 0.13 | 26,26,26,26                 | 0     |
| 84  | MG   | AS    | 3436 | 1/1   | 0.86 | 0.21 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3746 | 1/1   | 0.86 | 0.05 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3759 | 1/1   | 0.86 | 0.13 | 74,74,74,74                 | 0     |
| 84  | MG   | BK    | 201  | 1/1   | 0.86 | 0.11 | 73,73,73,73                 | 0     |
| 84  | MG   | B     | 1843 | 1/1   | 0.86 | 0.14 | 75,75,75,75                 | 0     |
| 84  | MG   | B     | 1882 | 1/1   | 0.86 | 0.20 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3815 | 1/1   | 0.86 | 0.17 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3754 | 1/1   | 0.86 | 0.10 | 106,106,106,106             | 0     |
| 84  | MG   | x     | 201  | 1/1   | 0.86 | 0.16 | 53,53,53,53                 | 0     |
| 84  | MG   | AS    | 3447 | 1/1   | 0.86 | 0.17 | 55,55,55,55                 | 0     |
| 84  | MG   | DH    | 201  | 1/1   | 0.86 | 0.07 | 53,53,53,53                 | 0     |
| 84  | MG   | 1     | 3760 | 1/1   | 0.86 | 0.13 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3671 | 1/1   | 0.86 | 0.10 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3420 | 1/1   | 0.86 | 0.15 | 21,21,21,21                 | 0     |
| 84  | MG   | AS    | 3550 | 1/1   | 0.86 | 0.20 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | B     | 1879 | 1/1   | 0.87 | 0.15 | 58,58,58,58                 | 0     |
| 84  | MG   | CM    | 1807 | 1/1   | 0.87 | 0.12 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3855 | 1/1   | 0.87 | 0.09 | 43,43,43,43                 | 0     |
| 84  | MG   | AS    | 3459 | 1/1   | 0.87 | 0.11 | 66,66,66,66                 | 0     |
| 84  | MG   | 1     | 3833 | 1/1   | 0.87 | 0.13 | 47,47,47,47                 | 0     |
| 84  | MG   | AS    | 3462 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3466 | 1/1   | 0.87 | 0.07 | 44,44,44,44                 | 0     |
| 84  | MG   | B     | 1840 | 1/1   | 0.87 | 0.23 | 47,47,47,47                 | 0     |
| 84  | MG   | 1     | 3667 | 1/1   | 0.87 | 0.15 | 37,37,37,37                 | 0     |
| 84  | MG   | AS    | 3768 | 1/1   | 0.87 | 0.10 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3715 | 1/1   | 0.87 | 0.16 | 47,47,47,47                 | 0     |
| 84  | MG   | 1     | 3649 | 1/1   | 0.87 | 0.07 | 85,85,85,85                 | 0     |
| 84  | MG   | AS    | 3417 | 1/1   | 0.87 | 0.21 | 47,47,47,47                 | 0     |
| 84  | MG   | u     | 201  | 1/1   | 0.87 | 0.13 | 83,83,83,83                 | 0     |
| 84  | MG   | 1     | 3862 | 1/1   | 0.87 | 0.23 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3838 | 1/1   | 0.87 | 0.10 | 53,53,53,53                 | 0     |
| 84  | MG   | CM    | 1842 | 1/1   | 0.87 | 0.16 | 67,67,67,67                 | 0     |
| 84  | MG   | 1     | 3792 | 1/1   | 0.87 | 0.11 | 150,150,150,150             | 0     |
| 84  | MG   | B     | 1819 | 1/1   | 0.87 | 0.12 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3539 | 1/1   | 0.87 | 0.15 | 53,53,53,53                 | 0     |
| 84  | MG   | 1     | 3780 | 1/1   | 0.87 | 0.07 | 103,103,103,103             | 0     |
| 84  | MG   | 1     | 3868 | 1/1   | 0.87 | 0.34 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3540 | 1/1   | 0.87 | 0.17 | 108,108,108,108             | 0     |
| 84  | MG   | 1     | 3686 | 1/1   | 0.87 | 0.09 | 103,103,103,103             | 0     |
| 84  | MG   | AS    | 3434 | 1/1   | 0.87 | 0.29 | 64,64,64,64                 | 0     |
| 84  | MG   | B     | 1827 | 1/1   | 0.87 | 0.17 | 61,61,61,61                 | 0     |
| 84  | MG   | AS    | 3636 | 1/1   | 0.87 | 0.13 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3637 | 1/1   | 0.87 | 0.10 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3671 | 1/1   | 0.87 | 0.12 | 75,75,75,75                 | 0     |
| 84  | MG   | AS    | 3640 | 1/1   | 0.87 | 0.12 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3738 | 1/1   | 0.87 | 0.20 | 67,67,67,67                 | 0     |
| 84  | MG   | Q     | 202  | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 84  | MG   | B     | 1863 | 1/1   | 0.87 | 0.17 | 53,53,53,53                 | 0     |
| 84  | MG   | 3     | 202  | 1/1   | 0.87 | 0.11 | 45,45,45,45                 | 0     |
| 84  | MG   | AS    | 3600 | 1/1   | 0.87 | 0.09 | 76,76,76,76                 | 0     |
| 84  | MG   | AS    | 3647 | 1/1   | 0.87 | 0.28 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3440 | 1/1   | 0.87 | 0.13 | 67,67,67,67                 | 0     |
| 84  | MG   | B     | 1870 | 1/1   | 0.87 | 0.12 | 63,63,63,63                 | 0     |
| 84  | MG   | BO    | 201  | 1/1   | 0.87 | 0.10 | 91,91,91,91                 | 0     |
| 84  | MG   | 1     | 3439 | 1/1   | 0.87 | 0.20 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3816 | 1/1   | 0.87 | 0.25 | 59,59,59,59                 | 0     |
| 84  | MG   | AS    | 3652 | 1/1   | 0.87 | 0.21 | 105,105,105,105             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3753 | 1/1   | 0.87 | 0.28 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3402 | 1/1   | 0.87 | 0.14 | 75,75,75,75                 | 0     |
| 84  | MG   | CM    | 1802 | 1/1   | 0.87 | 0.22 | 53,53,53,53                 | 0     |
| 84  | MG   | CM    | 1824 | 1/1   | 0.88 | 0.19 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3679 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3472 | 1/1   | 0.88 | 0.11 | 60,60,60,60                 | 0     |
| 84  | MG   | K     | 301  | 1/1   | 0.88 | 0.06 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3695 | 1/1   | 0.88 | 0.10 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3801 | 1/1   | 0.88 | 0.16 | 55,55,55,55                 | 0     |
| 84  | MG   | 1     | 3668 | 1/1   | 0.88 | 0.06 | 23,23,23,23                 | 0     |
| 84  | MG   | 1     | 3682 | 1/1   | 0.88 | 0.19 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3488 | 1/1   | 0.88 | 0.25 | 32,32,32,32                 | 0     |
| 84  | MG   | 1     | 3509 | 1/1   | 0.88 | 0.07 | 11,11,11,11                 | 0     |
| 84  | MG   | AS    | 3690 | 1/1   | 0.88 | 0.07 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3518 | 1/1   | 0.88 | 0.20 | 69,69,69,69                 | 0     |
| 84  | MG   | B     | 1883 | 1/1   | 0.88 | 0.08 | 47,47,47,47                 | 0     |
| 84  | MG   | 1     | 3829 | 1/1   | 0.88 | 0.11 | 42,42,42,42                 | 0     |
| 84  | MG   | 1     | 3459 | 1/1   | 0.88 | 0.21 | 43,43,43,43                 | 0     |
| 84  | MG   | AU    | 205  | 1/1   | 0.88 | 0.10 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3574 | 1/1   | 0.88 | 0.09 | 87,87,87,87                 | 0     |
| 84  | MG   | 1     | 3727 | 1/1   | 0.88 | 0.30 | 61,61,61,61                 | 0     |
| 84  | MG   | AS    | 3502 | 1/1   | 0.88 | 0.15 | 74,74,74,74                 | 0     |
| 84  | MG   | CM    | 1853 | 1/1   | 0.88 | 0.13 | 80,80,80,80                 | 0     |
| 84  | MG   | 1     | 3728 | 1/1   | 0.88 | 0.13 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3521 | 1/1   | 0.88 | 0.20 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3701 | 1/1   | 0.88 | 0.20 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3498 | 1/1   | 0.88 | 0.11 | 58,58,58,58                 | 0     |
| 84  | MG   | CM    | 1867 | 1/1   | 0.88 | 0.17 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3506 | 1/1   | 0.88 | 0.11 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3624 | 1/1   | 0.88 | 0.10 | 85,85,85,85                 | 0     |
| 84  | MG   | CM    | 1870 | 1/1   | 0.88 | 0.17 | 94,94,94,94                 | 0     |
| 84  | MG   | 1     | 3836 | 1/1   | 0.88 | 0.23 | 77,77,77,77                 | 0     |
| 84  | MG   | B     | 1822 | 1/1   | 0.88 | 0.16 | 105,105,105,105             | 0     |
| 84  | MG   | 6     | 201  | 1/1   | 0.88 | 0.17 | 53,53,53,53                 | 0     |
| 84  | MG   | AS    | 3419 | 1/1   | 0.88 | 0.18 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3629 | 1/1   | 0.88 | 0.27 | 43,43,43,43                 | 0     |
| 84  | MG   | AS    | 3548 | 1/1   | 0.88 | 0.11 | 91,91,91,91                 | 0     |
| 84  | MG   | 1     | 3588 | 1/1   | 0.88 | 0.12 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3514 | 1/1   | 0.88 | 0.22 | 53,53,53,53                 | 0     |
| 84  | MG   | AS    | 3760 | 1/1   | 0.88 | 0.14 | 67,67,67,67                 | 0     |
| 84  | MG   | CM    | 1801 | 1/1   | 0.88 | 0.23 | 41,41,41,41                 | 0     |
| 84  | MG   | AS    | 3763 | 1/1   | 0.88 | 0.19 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3526 | 1/1   | 0.88 | 0.09 | 103,103,103,103             | 0     |
| 84  | MG   | 1     | 3569 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3432 | 1/1   | 0.88 | 0.19 | 78,78,78,78                 | 0     |
| 84  | MG   | 1     | 3775 | 1/1   | 0.88 | 0.08 | 55,55,55,55                 | 0     |
| 84  | MG   | 1     | 3712 | 1/1   | 0.88 | 0.12 | 50,50,50,50                 | 0     |
| 85  | ZN   | DS    | 201  | 1/1   | 0.88 | 0.06 | 353,353,353,353             | 0     |
| 84  | MG   | B     | 1889 | 1/1   | 0.89 | 0.11 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3848 | 1/1   | 0.89 | 0.08 | 69,69,69,69                 | 0     |
| 84  | MG   | CM    | 1809 | 1/1   | 0.89 | 0.19 | 60,60,60,60                 | 0     |
| 84  | MG   | CM    | 1810 | 1/1   | 0.89 | 0.27 | 52,52,52,52                 | 0     |
| 84  | MG   | CM    | 1815 | 1/1   | 0.89 | 0.18 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3701 | 1/1   | 0.89 | 0.06 | 87,87,87,87                 | 0     |
| 84  | MG   | m     | 301  | 1/1   | 0.89 | 0.13 | 61,61,61,61                 | 0     |
| 84  | MG   | B     | 1847 | 1/1   | 0.89 | 0.13 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3658 | 1/1   | 0.89 | 0.12 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3432 | 1/1   | 0.89 | 0.20 | 92,92,92,92                 | 0     |
| 84  | MG   | B     | 1852 | 1/1   | 0.89 | 0.15 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3766 | 1/1   | 0.89 | 0.17 | 63,63,63,63                 | 0     |
| 83  | 3K5  | 1     | 3401 | 57/57 | 0.89 | 0.19 | 72,107,146,164              | 0     |
| 84  | MG   | 1     | 3520 | 1/1   | 0.89 | 0.15 | 95,95,95,95                 | 0     |
| 84  | MG   | 1     | 3447 | 1/1   | 0.89 | 0.07 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3775 | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3484 | 1/1   | 0.89 | 0.08 | 27,27,27,27                 | 0     |
| 84  | MG   | AS    | 3778 | 1/1   | 0.89 | 0.13 | 60,60,60,60                 | 0     |
| 84  | MG   | D     | 301  | 1/1   | 0.89 | 0.12 | 24,24,24,24                 | 0     |
| 84  | MG   | 1     | 3524 | 1/1   | 0.89 | 0.15 | 93,93,93,93                 | 0     |
| 84  | MG   | 1     | 3601 | 1/1   | 0.89 | 0.19 | 57,57,57,57                 | 0     |
| 84  | MG   | 1     | 3619 | 1/1   | 0.89 | 0.06 | 5,5,5,5                     | 0     |
| 84  | MG   | AS    | 3565 | 1/1   | 0.89 | 0.20 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3444 | 1/1   | 0.89 | 0.16 | 52,52,52,52                 | 0     |
| 84  | MG   | Q     | 201  | 1/1   | 0.89 | 0.20 | 110,110,110,110             | 0     |
| 84  | MG   | 1     | 3643 | 1/1   | 0.89 | 0.23 | 51,51,51,51                 | 0     |
| 84  | MG   | CM    | 1848 | 1/1   | 0.89 | 0.11 | 104,104,104,104             | 0     |
| 84  | MG   | CM    | 1849 | 1/1   | 0.89 | 0.13 | 67,67,67,67                 | 0     |
| 84  | MG   | y     | 203  | 1/1   | 0.89 | 0.20 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3675 | 1/1   | 0.89 | 0.14 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3554 | 1/1   | 0.89 | 0.04 | 65,65,65,65                 | 0     |
| 84  | MG   | 0     | 202  | 1/1   | 0.89 | 0.20 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3716 | 1/1   | 0.89 | 0.14 | 46,46,46,46                 | 0     |
| 84  | MG   | AS    | 3733 | 1/1   | 0.89 | 0.14 | 102,102,102,102             | 0     |
| 84  | MG   | CM    | 1866 | 1/1   | 0.89 | 0.17 | 83,83,83,83                 | 0     |
| 84  | MG   | B     | 1869 | 1/1   | 0.89 | 0.13 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3589 | 1/1   | 0.89 | 0.10 | 75,75,75,75                 | 0     |
| 84  | MG   | B     | 1871 | 1/1   | 0.89 | 0.09 | 40,40,40,40                 | 0     |
| 84  | MG   | 1     | 3410 | 1/1   | 0.89 | 0.21 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3435 | 1/1   | 0.89 | 0.14 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3407 | 1/1   | 0.89 | 0.09 | 83,83,83,83                 | 0     |
| 84  | MG   | AS    | 3473 | 1/1   | 0.89 | 0.21 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3629 | 1/1   | 0.89 | 0.12 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3409 | 1/1   | 0.89 | 0.17 | 86,86,86,86                 | 0     |
| 84  | MG   | AJ    | 101  | 1/1   | 0.89 | 0.22 | 100,100,100,100             | 0     |
| 84  | MG   | 1     | 3510 | 1/1   | 0.89 | 0.15 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3632 | 1/1   | 0.89 | 0.11 | 51,51,51,51                 | 0     |
| 84  | MG   | AS    | 3747 | 1/1   | 0.89 | 0.16 | 47,47,47,47                 | 0     |
| 84  | MG   | AS    | 3537 | 1/1   | 0.89 | 0.19 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3635 | 1/1   | 0.89 | 0.23 | 45,45,45,45                 | 0     |
| 84  | MG   | 4     | 201  | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 84  | MG   | AS    | 3595 | 1/1   | 0.89 | 0.12 | 72,72,72,72                 | 0     |
| 84  | MG   | B     | 1842 | 1/1   | 0.89 | 0.16 | 67,67,67,67                 | 0     |
| 85  | ZN   | AP    | 201  | 1/1   | 0.89 | 0.06 | 294,294,294,294             | 0     |
| 84  | MG   | CL    | 302  | 1/1   | 0.89 | 0.14 | 88,88,88,88                 | 0     |
| 85  | ZN   | h     | 201  | 1/1   | 0.89 | 0.09 | 285,285,285,285             | 0     |
| 84  | MG   | B     | 1887 | 1/1   | 0.89 | 0.09 | 81,81,81,81                 | 0     |
| 85  | ZN   | CJ    | 201  | 1/1   | 0.89 | 0.06 | 300,300,300,300             | 0     |
| 84  | MG   | 1     | 3798 | 1/1   | 0.89 | 0.05 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3462 | 1/1   | 0.90 | 0.15 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3456 | 1/1   | 0.90 | 0.10 | 31,31,31,31                 | 0     |
| 84  | MG   | 1     | 3611 | 1/1   | 0.90 | 0.15 | 81,81,81,81                 | 0     |
| 84  | MG   | 1     | 3421 | 1/1   | 0.90 | 0.13 | 48,48,48,48                 | 0     |
| 84  | MG   | AU    | 203  | 1/1   | 0.90 | 0.08 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3615 | 1/1   | 0.90 | 0.13 | 40,40,40,40                 | 0     |
| 84  | MG   | AS    | 3461 | 1/1   | 0.90 | 0.18 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3718 | 1/1   | 0.90 | 0.11 | 42,42,42,42                 | 0     |
| 84  | MG   | 1     | 3487 | 1/1   | 0.90 | 0.14 | 43,43,43,43                 | 0     |
| 84  | MG   | AS    | 3467 | 1/1   | 0.90 | 0.14 | 79,79,79,79                 | 0     |
| 84  | MG   | B     | 1877 | 1/1   | 0.90 | 0.13 | 47,47,47,47                 | 0     |
| 84  | MG   | AS    | 3590 | 1/1   | 0.90 | 0.06 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3669 | 1/1   | 0.90 | 0.11 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3471 | 1/1   | 0.90 | 0.21 | 41,41,41,41                 | 0     |
| 84  | MG   | AS    | 3632 | 1/1   | 0.90 | 0.11 | 85,85,85,85                 | 0     |
| 84  | MG   | 1     | 3600 | 1/1   | 0.90 | 0.18 | 55,55,55,55                 | 0     |
| 84  | MG   | B     | 1813 | 1/1   | 0.90 | 0.16 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3488 | 1/1   | 0.90 | 0.08 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3811 | 1/1   | 0.90 | 0.07 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3557 | 1/1   | 0.90 | 0.08 | 60,60,60,60                 | 0     |
| 84  | MG   | CM    | 1865 | 1/1   | 0.90 | 0.06 | 119,119,119,119             | 0     |
| 84  | MG   | 1     | 3812 | 1/1   | 0.90 | 0.16 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3513 | 1/1   | 0.90 | 0.22 | 64,64,64,64                 | 0     |
| 84  | MG   | AS    | 3480 | 1/1   | 0.90 | 0.13 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3766 | 1/1   | 0.90 | 0.13 | 47,47,47,47                 | 0     |
| 83  | 3K5  | AS    | 3401 | 57/57 | 0.90 | 0.15 | 82,121,151,184              | 0     |
| 84  | MG   | AS    | 3644 | 1/1   | 0.90 | 0.17 | 86,86,86,86                 | 0     |
| 84  | MG   | AS    | 3771 | 1/1   | 0.90 | 0.32 | 69,69,69,69                 | 0     |
| 84  | MG   | CM    | 1803 | 1/1   | 0.90 | 0.06 | 192,192,192,192             | 0     |
| 84  | MG   | 1     | 3549 | 1/1   | 0.90 | 0.19 | 66,66,66,66                 | 0     |
| 84  | MG   | 1     | 3729 | 1/1   | 0.90 | 0.04 | 56,56,56,56                 | 0     |
| 84  | MG   | CM    | 1808 | 1/1   | 0.90 | 0.06 | 61,61,61,61                 | 0     |
| 84  | MG   | AS    | 3487 | 1/1   | 0.90 | 0.15 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3779 | 1/1   | 0.90 | 0.08 | 66,66,66,66                 | 0     |
| 84  | MG   | AS    | 3732 | 1/1   | 0.90 | 0.10 | 85,85,85,85                 | 0     |
| 84  | MG   | AS    | 3782 | 1/1   | 0.90 | 0.17 | 72,72,72,72                 | 0     |
| 84  | MG   | CM    | 1820 | 1/1   | 0.90 | 0.15 | 68,68,68,68                 | 0     |
| 84  | MG   | 1     | 3424 | 1/1   | 0.90 | 0.07 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3706 | 1/1   | 0.90 | 0.10 | 60,60,60,60                 | 0     |
| 84  | MG   | DK    | 202  | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 0     |
| 84  | MG   | 3     | 207  | 1/1   | 0.90 | 0.12 | 48,48,48,48                 | 0     |
| 84  | MG   | 1     | 3453 | 1/1   | 0.90 | 0.25 | 67,67,67,67                 | 0     |
| 84  | MG   | 1     | 3471 | 1/1   | 0.90 | 0.09 | 40,40,40,40                 | 0     |
| 84  | MG   | CM    | 1828 | 1/1   | 0.90 | 0.15 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3428 | 1/1   | 0.90 | 0.27 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3633 | 1/1   | 0.90 | 0.24 | 27,27,27,27                 | 0     |
| 84  | MG   | B     | 1864 | 1/1   | 0.90 | 0.19 | 67,67,67,67                 | 0     |
| 86  | GET  | B     | 1851 | 34/34 | 0.90 | 0.09 | 105,127,149,167             | 0     |
| 84  | MG   | AS    | 3492 | 1/1   | 0.91 | 0.16 | 97,97,97,97                 | 0     |
| 84  | MG   | 1     | 3708 | 1/1   | 0.91 | 0.13 | 103,103,103,103             | 0     |
| 84  | MG   | 1     | 3590 | 1/1   | 0.91 | 0.24 | 57,57,57,57                 | 0     |
| 84  | MG   | r     | 301  | 1/1   | 0.91 | 0.09 | 48,48,48,48                 | 0     |
| 84  | MG   | AS    | 3619 | 1/1   | 0.91 | 0.10 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3455 | 1/1   | 0.91 | 0.11 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3491 | 1/1   | 0.91 | 0.29 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3578 | 1/1   | 0.91 | 0.12 | 52,52,52,52                 | 0     |
| 84  | MG   | 1     | 3561 | 1/1   | 0.91 | 0.11 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3772 | 1/1   | 0.91 | 0.09 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3450 | 1/1   | 0.91 | 0.20 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3502 | 1/1   | 0.91 | 0.20 | 53,53,53,53                 | 0     |
| 84  | MG   | B     | 1875 | 1/1   | 0.91 | 0.05 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3465 | 1/1   | 0.91 | 0.12 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3546 | 1/1   | 0.91 | 0.15 | 38,38,38,38                 | 0     |
| 84  | MG   | 1     | 3656 | 1/1   | 0.91 | 0.18 | 52,52,52,52                 | 0     |
| 84  | MG   | CM    | 1858 | 1/1   | 0.91 | 0.09 | 111,111,111,111             | 0     |
| 84  | MG   | AS    | 3510 | 1/1   | 0.91 | 0.13 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3620 | 1/1   | 0.91 | 0.10 | 49,49,49,49                 | 0     |
| 84  | MG   | 1     | 3448 | 1/1   | 0.91 | 0.15 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3513 | 1/1   | 0.91 | 0.08 | 47,47,47,47                 | 0     |
| 84  | MG   | AS    | 3594 | 1/1   | 0.91 | 0.11 | 104,104,104,104             | 0     |
| 84  | MG   | 1     | 3566 | 1/1   | 0.91 | 0.08 | 32,32,32,32                 | 0     |
| 84  | MG   | 1     | 3557 | 1/1   | 0.91 | 0.09 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3774 | 1/1   | 0.91 | 0.11 | 37,37,37,37                 | 0     |
| 84  | MG   | 1     | 3626 | 1/1   | 0.91 | 0.12 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3786 | 1/1   | 0.91 | 0.06 | 45,45,45,45                 | 0     |
| 84  | MG   | B     | 1824 | 1/1   | 0.91 | 0.14 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3727 | 1/1   | 0.91 | 0.06 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3851 | 1/1   | 0.91 | 0.21 | 76,76,76,76                 | 0     |
| 84  | MG   | 1     | 3666 | 1/1   | 0.91 | 0.09 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3627 | 1/1   | 0.91 | 0.34 | 46,46,46,46                 | 0     |
| 84  | MG   | CM    | 1817 | 1/1   | 0.91 | 0.07 | 190,190,190,190             | 0     |
| 84  | MG   | AS    | 3605 | 1/1   | 0.91 | 0.16 | 91,91,91,91                 | 0     |
| 84  | MG   | 1     | 3522 | 1/1   | 0.91 | 0.07 | 38,38,38,38                 | 0     |
| 84  | MG   | AS    | 3689 | 1/1   | 0.91 | 0.04 | 59,59,59,59                 | 0     |
| 84  | MG   | B     | 1890 | 1/1   | 0.91 | 0.12 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3442 | 1/1   | 0.91 | 0.21 | 22,22,22,22                 | 0     |
| 84  | MG   | 1     | 3452 | 1/1   | 0.91 | 0.15 | 63,63,63,63                 | 0     |
| 84  | MG   | CM    | 1827 | 1/1   | 0.91 | 0.10 | 35,35,35,35                 | 0     |
| 84  | MG   | 1     | 3612 | 1/1   | 0.91 | 0.12 | 74,74,74,74                 | 0     |
| 84  | MG   | AS    | 3694 | 1/1   | 0.91 | 0.18 | 45,45,45,45                 | 0     |
| 84  | MG   | B     | 1833 | 1/1   | 0.91 | 0.09 | 72,72,72,72                 | 0     |
| 84  | MG   | B     | 1894 | 1/1   | 0.91 | 0.07 | 98,98,98,98                 | 0     |
| 84  | MG   | AS    | 3450 | 1/1   | 0.91 | 0.16 | 47,47,47,47                 | 0     |
| 84  | MG   | AT    | 205  | 1/1   | 0.91 | 0.16 | 75,75,75,75                 | 0     |
| 84  | MG   | CM    | 1835 | 1/1   | 0.91 | 0.08 | 68,68,68,68                 | 0     |
| 84  | MG   | 1     | 3596 | 1/1   | 0.92 | 0.05 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3774 | 1/1   | 0.92 | 0.07 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3486 | 1/1   | 0.92 | 0.19 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3688 | 1/1   | 0.92 | 0.09 | 106,106,106,106             | 0     |
| 84  | MG   | 1     | 3422 | 1/1   | 0.92 | 0.14 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3690 | 1/1   | 0.92 | 0.11 | 61,61,61,61                 | 0     |
| 84  | MG   | B     | 1816 | 1/1   | 0.92 | 0.07 | 34,34,34,34                 | 0     |
| 84  | MG   | BI    | 301  | 1/1   | 0.92 | 0.05 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3672 | 1/1   | 0.92 | 0.11 | 63,63,63,63                 | 0     |
| 84  | MG   | 1     | 3512 | 1/1   | 0.92 | 0.15 | 53,53,53,53                 | 0     |
| 84  | MG   | 1     | 3781 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3416 | 1/1   | 0.92 | 0.15 | 41,41,41,41                 | 0     |
| 84  | MG   | 1     | 3757 | 1/1   | 0.92 | 0.07 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3503 | 1/1   | 0.92 | 0.16 | 70,70,70,70                 | 0     |
| 84  | MG   | y     | 202  | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |
| 84  | MG   | 1     | 3713 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 84  | MG   | CM    | 1860 | 1/1   | 0.92 | 0.18 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3866 | 1/1   | 0.92 | 0.14 | 86,86,86,86                 | 0     |
| 84  | MG   | AS    | 3772 | 1/1   | 0.92 | 0.06 | 59,59,59,59                 | 0     |
| 84  | MG   | CM    | 1863 | 1/1   | 0.92 | 0.14 | 70,70,70,70                 | 0     |
| 84  | MG   | AS    | 3639 | 1/1   | 0.92 | 0.05 | 60,60,60,60                 | 0     |
| 84  | MG   | B     | 1825 | 1/1   | 0.92 | 0.08 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3425 | 1/1   | 0.92 | 0.09 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3777 | 1/1   | 0.92 | 0.15 | 98,98,98,98                 | 0     |
| 84  | MG   | 1     | 3443 | 1/1   | 0.92 | 0.20 | 35,35,35,35                 | 0     |
| 84  | MG   | 1     | 3433 | 1/1   | 0.92 | 0.17 | 34,34,34,34                 | 0     |
| 84  | MG   | 1     | 3655 | 1/1   | 0.92 | 0.07 | 58,58,58,58                 | 0     |
| 84  | MG   | CM    | 1872 | 1/1   | 0.92 | 0.07 | 85,85,85,85                 | 0     |
| 84  | MG   | B     | 1866 | 1/1   | 0.92 | 0.12 | 47,47,47,47                 | 0     |
| 84  | MG   | CM    | 1812 | 1/1   | 0.92 | 0.08 | 152,152,152,152             | 0     |
| 84  | MG   | 1     | 3460 | 1/1   | 0.92 | 0.16 | 45,45,45,45                 | 0     |
| 84  | MG   | B     | 1830 | 1/1   | 0.92 | 0.07 | 79,79,79,79                 | 0     |
| 84  | MG   | 1     | 3577 | 1/1   | 0.92 | 0.07 | 48,48,48,48                 | 0     |
| 84  | MG   | CM    | 1818 | 1/1   | 0.92 | 0.21 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3721 | 1/1   | 0.92 | 0.09 | 86,86,86,86                 | 0     |
| 84  | MG   | 1     | 3844 | 1/1   | 0.92 | 0.18 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3507 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 84  | MG   | B     | 1873 | 1/1   | 0.92 | 0.21 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3551 | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 84  | MG   | 1     | 3540 | 1/1   | 0.92 | 0.11 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3477 | 1/1   | 0.92 | 0.17 | 41,41,41,41                 | 0     |
| 84  | MG   | P0    | 401  | 1/1   | 0.92 | 0.08 | 200,200,200,200             | 0     |
| 84  | MG   | AS    | 3617 | 1/1   | 0.92 | 0.17 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3533 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3404 | 1/1   | 0.92 | 0.12 | 22,22,22,22                 | 0     |
| 84  | MG   | k     | 403  | 1/1   | 0.92 | 0.08 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3495 | 1/1   | 0.92 | 0.24 | 41,41,41,41                 | 0     |
| 84  | MG   | AW    | 301  | 1/1   | 0.92 | 0.10 | 82,82,82,82                 | 0     |
| 84  | MG   | AS    | 3445 | 1/1   | 0.92 | 0.12 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3645 | 1/1   | 0.92 | 0.16 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3541 | 1/1   | 0.93 | 0.10 | 55,55,55,55                 | 0     |
| 84  | MG   | 1     | 3720 | 1/1   | 0.93 | 0.16 | 58,58,58,58                 | 0     |
| 84  | MG   | AS    | 3482 | 1/1   | 0.93 | 0.08 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3556 | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 84  | MG   | w     | 301  | 1/1   | 0.93 | 0.10 | 49,49,49,49                 | 0     |
| 84  | MG   | AS    | 3750 | 1/1   | 0.93 | 0.20 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3430 | 1/1   | 0.93 | 0.12 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3416 | 1/1   | 0.93 | 0.15 | 89,89,89,89                 | 0     |
| 84  | MG   | CM    | 1864 | 1/1   | 0.93 | 0.06 | 34,34,34,34                 | 0     |
| 84  | MG   | 3     | 205  | 1/1   | 0.93 | 0.18 | 32,32,32,32                 | 0     |
| 84  | MG   | 1     | 3724 | 1/1   | 0.93 | 0.07 | 74,74,74,74                 | 0     |
| 84  | MG   | CM    | 1819 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3490 | 1/1   | 0.93 | 0.05 | 62,62,62,62                 | 0     |
| 84  | MG   | T     | 201  | 1/1   | 0.93 | 0.11 | 121,121,121,121             | 0     |
| 84  | MG   | AS    | 3522 | 1/1   | 0.93 | 0.09 | 82,82,82,82                 | 0     |
| 84  | MG   | 1     | 3446 | 1/1   | 0.93 | 0.12 | 77,77,77,77                 | 0     |
| 84  | MG   | 1     | 3663 | 1/1   | 0.93 | 0.07 | 69,69,69,69                 | 0     |
| 84  | MG   | B     | 1817 | 1/1   | 0.93 | 0.25 | 56,56,56,56                 | 0     |
| 84  | MG   | AS    | 3761 | 1/1   | 0.93 | 0.14 | 89,89,89,89                 | 0     |
| 84  | MG   | 1     | 3857 | 1/1   | 0.93 | 0.13 | 92,92,92,92                 | 0     |
| 84  | MG   | 1     | 3631 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 84  | MG   | AS    | 3559 | 1/1   | 0.93 | 0.19 | 71,71,71,71                 | 0     |
| 84  | MG   | AS    | 3728 | 1/1   | 0.93 | 0.06 | 55,55,55,55                 | 0     |
| 84  | MG   | AS    | 3405 | 1/1   | 0.93 | 0.22 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3561 | 1/1   | 0.93 | 0.07 | 78,78,78,78                 | 0     |
| 84  | MG   | AS    | 3769 | 1/1   | 0.93 | 0.07 | 61,61,61,61                 | 0     |
| 84  | MG   | AS    | 3501 | 1/1   | 0.93 | 0.07 | 52,52,52,52                 | 0     |
| 84  | MG   | 1     | 3436 | 1/1   | 0.93 | 0.14 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3664 | 1/1   | 0.93 | 0.13 | 61,61,61,61                 | 0     |
| 84  | MG   | 1     | 3773 | 1/1   | 0.93 | 0.12 | 62,62,62,62                 | 0     |
| 84  | MG   | AS    | 3736 | 1/1   | 0.93 | 0.21 | 47,47,47,47                 | 0     |
| 84  | MG   | 1     | 3822 | 1/1   | 0.93 | 0.09 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3467 | 1/1   | 0.93 | 0.05 | 36,36,36,36                 | 0     |
| 84  | MG   | 1     | 3843 | 1/1   | 0.93 | 0.13 | 71,71,71,71                 | 0     |
| 84  | MG   | B     | 1848 | 1/1   | 0.93 | 0.10 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3525 | 1/1   | 0.93 | 0.14 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3475 | 1/1   | 0.93 | 0.21 | 16,16,16,16                 | 0     |
| 84  | MG   | 1     | 3657 | 1/1   | 0.93 | 0.09 | 69,69,69,69                 | 0     |
| 84  | MG   | 1     | 3719 | 1/1   | 0.93 | 0.10 | 74,74,74,74                 | 0     |
| 84  | MG   | 1     | 3469 | 1/1   | 0.94 | 0.09 | 31,31,31,31                 | 0     |
| 84  | MG   | AS    | 3499 | 1/1   | 0.94 | 0.04 | 70,70,70,70                 | 0     |
| 84  | MG   | 1     | 3634 | 1/1   | 0.94 | 0.22 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | 1     | 3483 | 1/1   | 0.94 | 0.08 | 112,112,112,112             | 0     |
| 84  | MG   | AS    | 3457 | 1/1   | 0.94 | 0.16 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3582 | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3622 | 1/1   | 0.94 | 0.05 | 72,72,72,72                 | 0     |
| 84  | MG   | 1     | 3608 | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 0     |
| 84  | MG   | B     | 1836 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 0     |
| 84  | MG   | 1     | 3429 | 1/1   | 0.94 | 0.14 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3840 | 1/1   | 0.94 | 0.09 | 67,67,67,67                 | 0     |
| 84  | MG   | CM    | 1852 | 1/1   | 0.94 | 0.14 | 37,37,37,37                 | 0     |
| 84  | MG   | 1     | 3445 | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 84  | MG   | CM    | 1855 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 84  | MG   | AS    | 3589 | 1/1   | 0.94 | 0.19 | 65,65,65,65                 | 0     |
| 84  | MG   | AS    | 3424 | 1/1   | 0.94 | 0.09 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3723 | 1/1   | 0.94 | 0.10 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3549 | 1/1   | 0.94 | 0.09 | 60,60,60,60                 | 0     |
| 84  | MG   | 1     | 3442 | 1/1   | 0.94 | 0.14 | 45,45,45,45                 | 0     |
| 84  | MG   | 1     | 3409 | 1/1   | 0.94 | 0.06 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3773 | 1/1   | 0.94 | 0.12 | 96,96,96,96                 | 0     |
| 84  | MG   | B     | 1874 | 1/1   | 0.94 | 0.12 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3613 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 84  | MG   | AS    | 3430 | 1/1   | 0.94 | 0.17 | 51,51,51,51                 | 0     |
| 84  | MG   | B     | 1876 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3710 | 1/1   | 0.94 | 0.13 | 42,42,42,42                 | 1     |
| 84  | MG   | 1     | 3531 | 1/1   | 0.94 | 0.12 | 84,84,84,84                 | 0     |
| 84  | MG   | R     | 203  | 1/1   | 0.94 | 0.14 | 59,59,59,59                 | 0     |
| 84  | MG   | AS    | 3781 | 1/1   | 0.94 | 0.03 | 58,58,58,58                 | 0     |
| 84  | MG   | 1     | 3676 | 1/1   | 0.94 | 0.14 | 65,65,65,65                 | 0     |
| 84  | MG   | AS    | 3604 | 1/1   | 0.94 | 0.13 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3826 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 84  | MG   | 0     | 204  | 1/1   | 0.94 | 0.10 | 77,77,77,77                 | 0     |
| 84  | MG   | AS    | 3483 | 1/1   | 0.94 | 0.08 | 103,103,103,103             | 0     |
| 84  | MG   | B     | 1849 | 1/1   | 0.94 | 0.09 | 91,91,91,91                 | 0     |
| 84  | MG   | 2     | 201  | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3564 | 1/1   | 0.94 | 0.14 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3808 | 1/1   | 0.94 | 0.09 | 144,144,144,144             | 0     |
| 84  | MG   | AS    | 3404 | 1/1   | 0.94 | 0.04 | 41,41,41,41                 | 0     |
| 84  | MG   | 1     | 3574 | 1/1   | 0.94 | 0.05 | 41,41,41,41                 | 0     |
| 84  | MG   | 1     | 3679 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 84  | MG   | 1     | 3854 | 1/1   | 0.94 | 0.07 | 81,81,81,81                 | 0     |
| 84  | MG   | AS    | 3702 | 1/1   | 0.94 | 0.07 | 66,66,66,66                 | 0     |
| 84  | MG   | AU    | 201  | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 84  | MG   | 1     | 3831 | 1/1   | 0.94 | 0.10 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AU    | 204  | 1/1   | 0.94 | 0.11 | 82,82,82,82                 | 0     |
| 84  | MG   | CM    | 1833 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 84  | MG   | AS    | 3494 | 1/1   | 0.94 | 0.06 | 105,105,105,105             | 0     |
| 84  | MG   | AP    | 202  | 1/1   | 0.94 | 0.16 | 49,49,49,49                 | 0     |
| 84  | MG   | 1     | 3456 | 1/1   | 0.94 | 0.19 | 47,47,47,47                 | 0     |
| 84  | MG   | CM    | 1837 | 1/1   | 0.94 | 0.16 | 62,62,62,62                 | 0     |
| 84  | MG   | 1     | 3664 | 1/1   | 0.94 | 0.24 | 40,40,40,40                 | 0     |
| 86  | GET  | CM    | 1822 | 34/34 | 0.94 | 0.12 | 107,119,148,157             | 0     |
| 84  | MG   | B     | 1865 | 1/1   | 0.95 | 0.19 | 65,65,65,65                 | 0     |
| 84  | MG   | CM    | 1814 | 1/1   | 0.95 | 0.08 | 127,127,127,127             | 0     |
| 84  | MG   | AS    | 3449 | 1/1   | 0.95 | 0.05 | 39,39,39,39                 | 0     |
| 84  | MG   | 1     | 3777 | 1/1   | 0.95 | 0.18 | 29,29,29,29                 | 0     |
| 84  | MG   | F     | 301  | 1/1   | 0.95 | 0.13 | 77,77,77,77                 | 0     |
| 84  | MG   | BE    | 301  | 1/1   | 0.95 | 0.10 | 59,59,59,59                 | 0     |
| 84  | MG   | AS    | 3598 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 84  | MG   | AS    | 3452 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |
| 84  | MG   | 0     | 203  | 1/1   | 0.95 | 0.04 | 33,33,33,33                 | 0     |
| 84  | MG   | 1     | 3465 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3476 | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 84  | MG   | BQ    | 201  | 1/1   | 0.95 | 0.18 | 54,54,54,54                 | 0     |
| 84  | MG   | L     | 201  | 1/1   | 0.95 | 0.25 | 55,55,55,55                 | 0     |
| 84  | MG   | AS    | 3438 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 84  | MG   | AS    | 3479 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 84  | MG   | 1     | 3438 | 1/1   | 0.95 | 0.14 | 75,75,75,75                 | 0     |
| 84  | MG   | 1     | 3616 | 1/1   | 0.95 | 0.09 | 65,65,65,65                 | 0     |
| 84  | MG   | 1     | 3501 | 1/1   | 0.95 | 0.14 | 64,64,64,64                 | 0     |
| 84  | MG   | B     | 1805 | 1/1   | 0.95 | 0.11 | 38,38,38,38                 | 0     |
| 84  | MG   | AS    | 3566 | 1/1   | 0.95 | 0.05 | 55,55,55,55                 | 0     |
| 84  | MG   | B     | 1837 | 1/1   | 0.95 | 0.08 | 57,57,57,57                 | 0     |
| 84  | MG   | 1     | 3861 | 1/1   | 0.95 | 0.08 | 54,54,54,54                 | 0     |
| 84  | MG   | AS    | 3463 | 1/1   | 0.95 | 0.08 | 41,41,41,41                 | 0     |
| 84  | MG   | 1     | 3473 | 1/1   | 0.95 | 0.10 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3413 | 1/1   | 0.95 | 0.15 | 44,44,44,44                 | 0     |
| 84  | MG   | AS    | 3593 | 1/1   | 0.95 | 0.10 | 68,68,68,68                 | 0     |
| 84  | MG   | AS    | 3661 | 1/1   | 0.96 | 0.10 | 66,66,66,66                 | 0     |
| 84  | MG   | B     | 1853 | 1/1   | 0.96 | 0.14 | 47,47,47,47                 | 0     |
| 84  | MG   | AS    | 3414 | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 84  | MG   | B     | 1808 | 1/1   | 0.96 | 0.03 | 57,57,57,57                 | 0     |
| 84  | MG   | AS    | 3464 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 84  | MG   | 1     | 3784 | 1/1   | 0.96 | 0.12 | 67,67,67,67                 | 0     |
| 84  | MG   | AS    | 3706 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 84  | MG   | AS    | 3418 | 1/1   | 0.96 | 0.22 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 84  | MG   | AS    | 3687 | 1/1   | 0.96 | 0.07 | 85,85,85,85                 | 0     |
| 84  | MG   | CM    | 1851 | 1/1   | 0.96 | 0.05 | 49,49,49,49                 | 0     |
| 84  | MG   | AU    | 202  | 1/1   | 0.96 | 0.05 | 60,60,60,60                 | 0     |
| 84  | MG   | AS    | 3730 | 1/1   | 0.96 | 0.12 | 46,46,46,46                 | 0     |
| 84  | MG   | 1     | 3739 | 1/1   | 0.96 | 0.10 | 98,98,98,98                 | 0     |
| 84  | MG   | AS    | 3468 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 84  | MG   | B     | 1881 | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 84  | MG   | AS    | 3470 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 84  | MG   | 3     | 203  | 1/1   | 0.96 | 0.20 | 54,54,54,54                 | 0     |
| 84  | MG   | CM    | 1804 | 1/1   | 0.96 | 0.05 | 48,48,48,48                 | 0     |
| 84  | MG   | B     | 1801 | 1/1   | 0.96 | 0.26 | 46,46,46,46                 | 0     |
| 84  | MG   | 3     | 204  | 1/1   | 0.96 | 0.16 | 30,30,30,30                 | 0     |
| 84  | MG   | 1     | 3852 | 1/1   | 0.96 | 0.09 | 71,71,71,71                 | 0     |
| 84  | MG   | 1     | 3464 | 1/1   | 0.96 | 0.08 | 8,8,8,8                     | 0     |
| 84  | MG   | 1     | 3653 | 1/1   | 0.96 | 0.15 | 30,30,30,30                 | 0     |
| 85  | ZN   | DN    | 201  | 1/1   | 0.96 | 0.05 | 125,125,125,125             | 0     |
| 84  | MG   | CM    | 1811 | 1/1   | 0.96 | 0.09 | 59,59,59,59                 | 0     |
| 84  | MG   | 1     | 3419 | 1/1   | 0.96 | 0.03 | 49,49,49,49                 | 0     |
| 84  | MG   | 1     | 3407 | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |
| 84  | MG   | AS    | 3427 | 1/1   | 0.97 | 0.11 | 39,39,39,39                 | 0     |
| 84  | MG   | 1     | 3696 | 1/1   | 0.97 | 0.09 | 39,39,39,39                 | 0     |
| 84  | MG   | 1     | 3660 | 1/1   | 0.97 | 0.14 | 35,35,35,35                 | 0     |
| 84  | MG   | CM    | 1806 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 84  | MG   | CM    | 1859 | 1/1   | 0.97 | 0.15 | 46,46,46,46                 | 0     |
| 85  | ZN   | AK    | 101  | 1/1   | 0.97 | 0.06 | 115,115,115,115             | 0     |
| 84  | MG   | AS    | 3415 | 1/1   | 0.97 | 0.16 | 81,81,81,81                 | 0     |
| 84  | MG   | 1     | 3621 | 1/1   | 0.97 | 0.07 | 56,56,56,56                 | 0     |
| 85  | ZN   | f     | 101  | 1/1   | 0.97 | 0.09 | 125,125,125,125             | 0     |
| 84  | MG   | AS    | 3448 | 1/1   | 0.97 | 0.09 | 73,73,73,73                 | 0     |
| 84  | MG   | AS    | 3531 | 1/1   | 0.97 | 0.13 | 86,86,86,86                 | 1     |
| 85  | ZN   | CE    | 101  | 1/1   | 0.97 | 0.05 | 128,128,128,128             | 0     |
| 84  | MG   | 1     | 3652 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 84  | MG   | 1     | 3437 | 1/1   | 0.97 | 0.08 | 49,49,49,49                 | 0     |
| 85  | ZN   | DQ    | 101  | 1/1   | 0.97 | 0.08 | 121,121,121,121             | 0     |
| 84  | MG   | CM    | 1813 | 1/1   | 0.97 | 0.07 | 168,168,168,168             | 0     |
| 84  | MG   | CM    | 1839 | 1/1   | 0.97 | 0.05 | 50,50,50,50                 | 0     |
| 84  | MG   | 1     | 3736 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 84  | MG   | AS    | 3762 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 85  | ZN   | AN    | 101  | 1/1   | 0.98 | 0.05 | 110,110,110,110             | 0     |
| 84  | MG   | AS    | 3493 | 1/1   | 0.98 | 0.14 | 36,36,36,36                 | 0     |
| 85  | ZN   | c     | 201  | 1/1   | 0.98 | 0.04 | 132,132,132,132             | 0     |
| 84  | MG   | CM    | 1854 | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |

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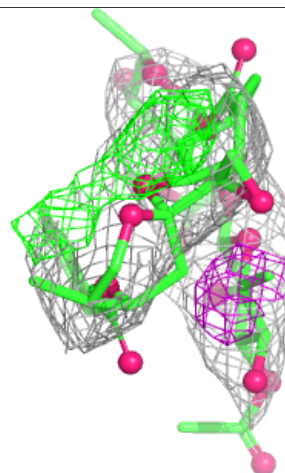
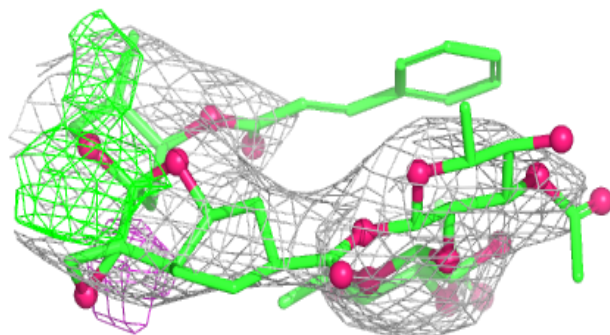
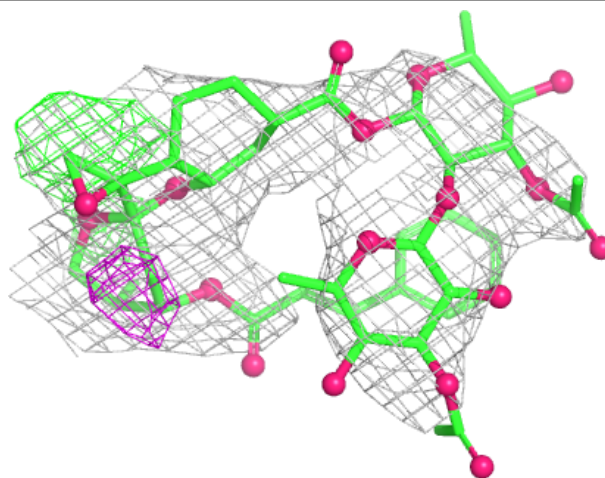
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 85  | ZN   | CK    | 101 | 1/1   | 0.99 | 0.03 | 151,151,151,151             | 0     |
| 85  | ZN   | CH    | 101 | 1/1   | 0.99 | 0.09 | 117,117,117,117             | 0     |
| 85  | ZN   | AQ    | 101 | 1/1   | 0.99 | 0.08 | 128,128,128,128             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

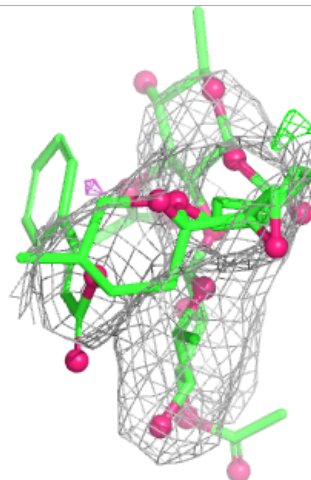
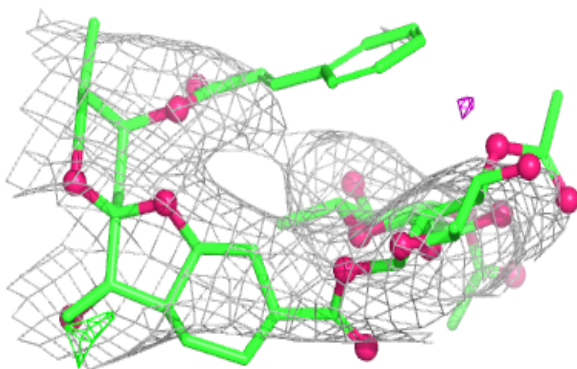
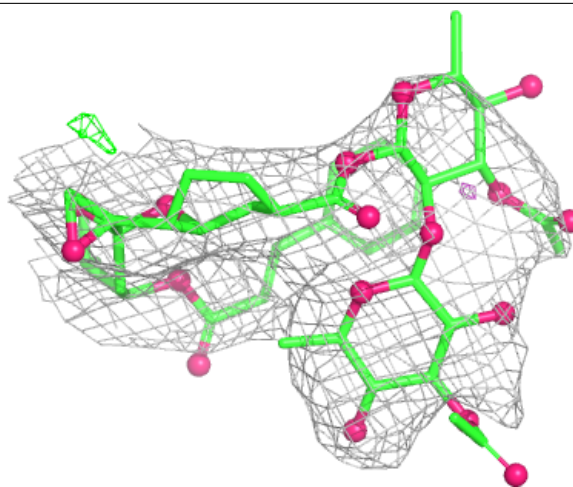
**Electron density around 3K5 1 3401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 3K5 AS 3401:**

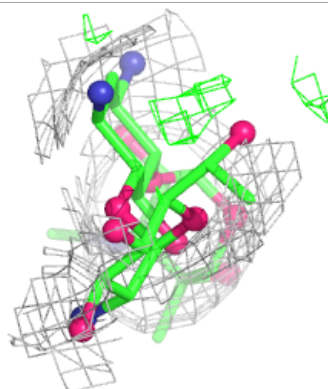
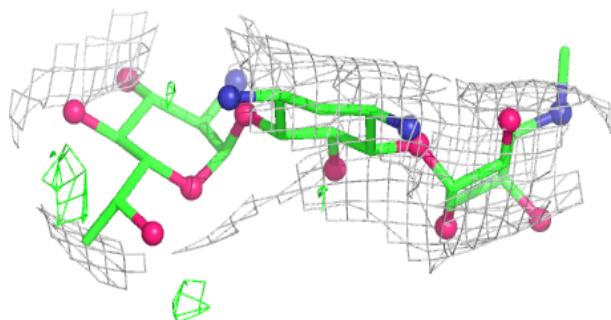
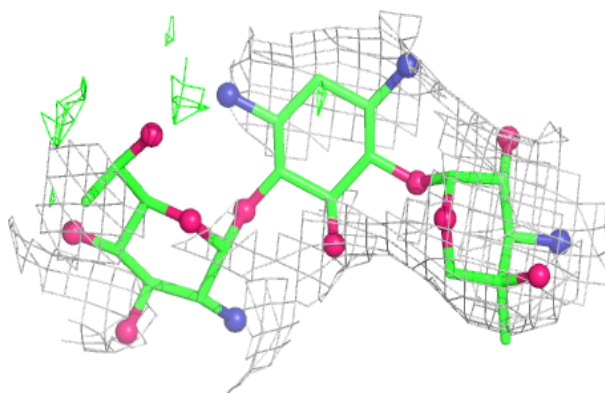
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



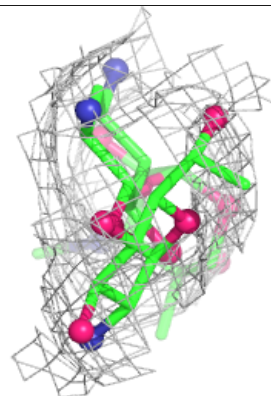
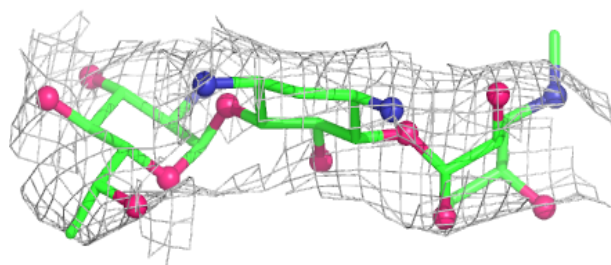
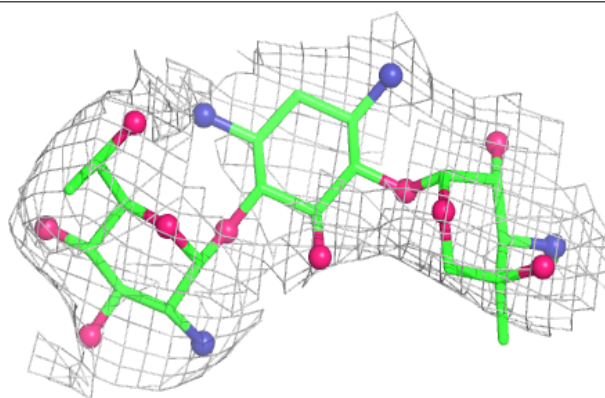


**Electron density around GET B 1851:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GET CM 1822:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.